Attorney Docket No.: PR60689USw

Amendments to the Claims:

Please amend the claims as follows:

(Currently Amended) A compound of formula (I)

or a sall including salts, solvates, and physiologically functional derivatives thereof, wherein

R' is -(Q'), R3;

Q¹ is C₁-C₉ alkylene;

x is 0 or 1;

R⁶ is H_ralkyl_ralkenyl, alkynyl, haloalkyl, or cycloalkyl <u>CF₂ or cyclopropyl</u>;

 R^2 is $-(Q^3)-(Q^4)-R^6$, or $-(Q^3)-CN$;

Q' is C.-C. alkylene;

Q4 is -C(O)-, -C(S)-, or -C(NR7)-,

R? is H or alkyl;

 \mathbb{R}^6 is $\underline{C_1}$, $\underline{C_6}$ alkeryl, $\underline{C_2}$, $\underline{C_6}$ alkynyl, hydroxy, $\underline{C_1}$, $\underline{C_6}$ alkoxy, anyloxy obenoxy.

benzyloxy, or -N(R8)(R8)

 R^8 and R^9 each independently are H, hydroxy, $\underline{C_1 \cdot C_0}$ alkyl, $\underline{C_2 \cdot C_0}$ alkenyl, $\underline{C_2 \cdot C_0}$ alkynyl, $-(Q^5)_7 \cdot \underline{C_2 \cdot C_0}$ cycloalkyl, $-N(R^{10})(R^{11})$, or R^8 and R^9 combine with the nitrogen atom to which they are attached to form an optionally substituted 4 to 8 membered ring that may contain additional heteroatoms and may contain one or more degrees of unsaturation;

Q⁵ is C₁-C₅ alkylene;

y is 0 or 1;

R¹⁰ and R¹¹ each independently are H or C₁+C₅ alkyl;

R3 is -CN, -NO2, or halogen; and

R* is -CN, -NO₂, halogen, C₂-C₆ haloalkyl, C₂-C₆ alkyl, C₂-C₆ alkenyl, C₂-C₆ alkynyl,

hydroxyl, C.-C. alkoxy, aryl-aryloxy phenyl, naphthyl, phenoxy or bebenzyloxy.

2-7. (Cancelled)

(Original) The compound of claim 1 wherein R³ is -CN.

Page 2 of 9

Author Search

=> FILE HCAPLUS

FILE 'HCAPLUS' ENTERED AT 10:21:14 ON 26 SEP 2008
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FILE COVERS 1907 - 26 Sep 2008 VOL 149 ISS 14 FILE LAST UPDATED: 25 Sep 2008 (20080925/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D STAT QUE L34 L1 STR

G2³ Cv ¹

 $Ak^2 G1$

G3 [02], [03]

G4

G5

G6 CN, NO2, X

Structure attributes must be viewed using STN Express query preparation.

L3 774 SEA FILE=REGISTRY SSS FUL L1

L4 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

L10 STR

 $G2^3$ Cy^1

 $Ak\frac{2}{G1}$

Structure attributes must be viewed using STN Express query preparation.

L12 395 SEA FILE=REGISTRY SUB=L3 SSS FUL L10
L13 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L12
L14 STR

 $G2^3$ Cy 1

 $Ak_{-}^{2}G1$

Structure attributes must be viewed using STN Express query preparation.

L16 SCR 342 OR 286

L17 2 SEA FILE=REGISTRY SSS SAM L16 AND L14

L27 62 SEA FILE=HCAPLUS ABB=ON PLU=ON TURNBULL P?/AU L28 17 SEA FILE=HCAPLUS ABB=ON PLU=ON CADILLA R?/AU

```
L29 675 SEA FILE=HCAPLUS ABB=ON PLU=ON COWAN D?/AU
L30 250 SEA FILE=HCAPLUS ABB=ON PLU=ON LARKIN A?/AU
L31 71 SEA FILE=HCAPLUS ABB=ON PLU=ON KALDOR I?/AU
L32 479 SEA FILE=HCAPLUS ABB=ON PLU=ON STEWART E?/AU
L33 1513 SEA FILE=HCAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29 OR L30 OR
L31 OR L32)
L34 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND (L4 OR L17 OR L13)
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=> FILE WPIX

FILE 'WPIX' ENTERED AT 10:21:27 ON 26 SEP 2008 COPYRIGHT (C) 2008 THOMSON REUTERS

FILE LAST UPDATED: 20 SEP 2008 <20080920/UP>
MOST RECENT UPDATE: 200860 <200860/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
>>> Now containing more than 1.1 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to the end of
June 2008. No update date (UP) has been created for the
reclassified documents, but they can be identified by
20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC,
20071130/UPIC, 20080401/UPIC and 20080701/UPIC.
ECLA reclassifications to June and US national classifications to
the end of April 2008 have also been loaded. Update dates
20080401 and 20080701/UPEC and /UPNC have been assigned to these. <<</pre>

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>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

'BI, ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D STAT QUE L38 L8 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
L27
           62 SEA FILE=HCAPLUS ABB=ON PLU=ON TURNBULL P?/AU
L28
           17 SEA FILE=HCAPLUS ABB=ON PLU=ON CADILLA R?/AU
L29
           675 SEA FILE=HCAPLUS ABB=ON PLU=ON COWAN D?/AU
L30
          250 SEA FILE=HCAPLUS ABB=ON PLU=ON LARKIN A?/AU
           71 SEA FILE=HCAPLUS ABB=ON PLU=ON KALDOR I?/AU
L31
L32
           479 SEA FILE=HCAPLUS ABB=ON PLU=ON STEWART E?/AU
L33
          1513 SEA FILE=HCAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29 OR L30 OR
              L31 OR L32)
L36
          109 SEA FILE=WPIX SSS FUL L8
            2 SEA FILE=WPIX ABB=ON PLU=ON L36/DCR
L37
L38
            2 SEA FILE=WPIX ABB=ON PLU=ON L33 AND L37
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Serial No.:10/598,508 => DUP REM L34 L38 FILE 'HCAPLUS' ENTERED AT 10:21:37 ON 26 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS) FILE 'WPIX' ENTERED AT 10:21:37 ON 26 SEP 2008 COPYRIGHT (C) 2008 THOMSON REUTERS PROCESSING COMPLETED FOR L34 PROCESSING COMPLETED FOR L38 6 DUP REM L34 L38 (2 DUPLICATES REMOVED) L41 ANSWERS '1-6' FROM FILE HCAPLUS => D IBIB ED ABS HITSTR 1-6 L41 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1 ACCESSION NUMBER: 2006:1122964 HCAPLUS <u>Full-text</u> DOCUMENT NUMBER: 145:455269 TITLE: Preparation of N-cyanoaryl amino acid amides for treating endometriosis or uterine fibroids Jones, David G.; Kaldor, Istvan; Liang, Xi; INVENTOR(S): Turnbull, Philip Stewart; Hammond, Marlys; Kallander, Lara S.; Thompson, Scott Kevin; Washburn, David PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA PCT Int. Appl., 71pp. SOURCE: CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

	PA:	CENT 1	NO.			KIND		DATE			APPLICATION NO.					D.	CA, CH, GB, GD, KP, KR, MW, MX, SD, SE, UZ, VC, HU, IE, BF, BJ, BW, GH, AZ, BY, 20060414 HU, IE, TR, AL,		
		2006		A2 A3		20061026 20070531			WO 2	006-		20060414							
		W: AE, AG,		AL,	AM,				BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
						•		•		•	•		•						
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,	
			KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	
			MZ,	NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	
			SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	
			VN,	YU,	ZA,	ZM,	ZW												
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			IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG,	BW,	GH,	
			GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	${\sf TZ}$,	UG,	ZM,	ZW,	ΑM,	ΑZ,	BY,	
			KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑP,	EA,	EP,	OA							
	EP	? 1871379						20080102											
		R:																	
			IS,	IT,	LI,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	AL,	
			BA,	HR,	MK,	YU													
	JP 2008536868					Τ		2008		JP 2	008-	50679							
	US 20080194536							2008	0814		US 2	007-	9115	20071015					
PRIOF	RIT	APP:	LN.	INFO	.:						US 2005-671592P					P 20050415			
											WO 2006-US14286					W 20060414			

OTHER SOURCE(S): MARPAT 145:455269

ED Entered STN: 27 Oct 2006

AB The invention relates to amino acid amides NC-Ar-N(CHR1R1')CR2R2'CONR3R3' [Ar is Ph or naphthyl which may be further substituted; R1, R1' are independently H, (un)substituted alkyl, cycloalkyl, aryl, heteroaryl, or together form a cycloalkyl or cycloalkenyl group; R2, R2' are independently H, (un)substituted alkyl, cycloalkyl, or R4(CH2)m-X-, where R4 is cycloalkyl, Ph, or pyridyl, m is 0-4, and X is a bond, O, or S; R3, R3' are independently (un)substituted alkyl, alkenyl, propargyl; or NR3R3' is heterocycloalkyl (with provisos)] or their pharmaceutically-acceptable salts and their use for treating endometriosis or uterine fibroids. Thus, N2-[(2-chlorophenyl)methyl]-N2-[4-cyano-3-(trifluoromethyl)phenyl]-N1,N1- dimethyl-L-alaninamide was prepared via amidation, arylation, and alkylation reactions. One hundred twenty-two synthesized compds. showed IC50 < 10 μM in the PR binding assay.

```
913288-02-5P 913288-03-6P 913288-04-7P
ΙT
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     913288-08-1P 913288-09-2P 913288-10-5P
     913288-11-6P 913288-12-7P 913288-13-8P
     913288-14-9P 913288-15-0P 913288-16-1P
     913288-17-2P 913288-18-3P 913288-19-4P
     913288-20-7P 913288-21-8P 913288-22-9P
     913288-23-0P 913288-24-1P 913288-25-2P
     913288-26-3P 913288-27-4P 913288-28-5P
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     913288-35-4P 913288-36-5P 913288-37-6P
     913288-38-7P 913288-39-8P 913288-40-1P
     913288-41-2P 913288-42-3P 913288-43-4P
     913288-44-5P 913288-45-6P 913288-46-7P
     913288-47-8P 913288-48-9P 913288-49-0P
     913288-50-3P 913288-51-4P 913288-52-5P
     913288-53-6P 913288-54-7P 913288-58-1P
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-cyanoaryl amino acid amides for treating endometriosis or uterine fibroids)

RN 913288-02-5 HCAPLUS

CN Pentanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

RN 913288-03-6 HCAPLUS
CN Hexanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

RN 913288-04-7 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-bis(2-methylpropyl)- (CA INDEX NAME)

RN 913288-05-8 HCAPLUS

CN Propanamide, N,N-dibutyl-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 913288-06-9 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(1,1-dimethylethyl)-N-methyl- (CA INDEX NAME)

RN 913288-07-0 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propyn-1-yl- (CA INDEX NAME)

RN 913288-08-1 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-propyl- (CA INDEX NAME)

RN 913288-09-2 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-(1-methylethyl)- (CA INDEX NAME)

RN 913288-10-5 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-methyl- (CA INDEX NAME)

RN 913288-11-6 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dipropyl- (CA INDEX NAME)

RN 913288-12-7 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-diethyl- (CA INDEX NAME)

RN 913288-13-8 HCAPLUS

CN Benzonitrile, 4-[[1-methyl-2-oxo-2-(1-piperidinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

CN Benzonitrile, 4-[[2-(1-azetidinyl)-1-methyl-2-oxoethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-15-0 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-propyl- (CA INDEX NAME)

RN 913288-16-1 HCAPLUS

CN Propanamide, N-butyl-N-(cyanomethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

$$CF_3$$
 Me
 $CH-C-N-Bu-n$
 F_3C-CH_2
 CH_2-CN

RN 913288-17-2 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(2-methoxyethyl)-N-propyl- (CA INDEX NAME)

RN 913288-18-3 HCAPLUS
CN Propanamide, N,N-bis(cyanomethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

$$CN$$
 CF_3
 Me
 N
 CH
 CH
 CN
 CH_2
 CN
 CH_2
 CN
 CH_2
 CN
 CH_2
 CN

RN 913288-19-4 HCAPLUS

CN Benzonitrile, 4-[[1-methyl-2-(4-morpholinyl)-2-oxoethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-20-7 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(cyclopropylmethyl)-N-propyl- (CA INDEX NAME)

RN 913288-21-8 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl-N-methyl- (CA INDEX NAME)

RN 913288-22-9 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)

RN 913288-23-0 HCAPLUS

CN Benzonitrile, 4-[[1-methyl-2-oxo-2-(4-thiomorpholinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-24-1 HCAPLUS

CN Propanamide, N-(2-cyanoethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 913288-25-2 HCAPLUS

CN Benzonitrile, 4-[[1-methyl-2-oxo-2-(1-pyrrolidinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-26-3 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-(1-methylethyl)- (CA INDEX NAME)

RN 913288-27-4 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-di-2-propen-1-yl- (CA INDEX NAME)

RN 913288-28-5 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propen-1-yl- (CA INDEX NAME)

RN 913288-29-6 HCAPLUS

CN Butanamide, N,N-dibutyl-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 913288-30-9 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(1,1-dimethylethyl)-N-methyl- (CA INDEX NAME)

$$CN$$
 $CF3$
 N
 CH
 Et
 F_3C
 CH_2
 CH_2
 CH
 Me

RN 913288-31-0 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propyn-1-yl- (CA INDEX NAME)

RN 913288-32-1 HCAPLUS
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-propyl- (CA INDEX NAME)

RN 913288-33-2 HCAPLUS
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-(1-methylethyl)- (CA INDEX NAME)

RN 913288-34-3 HCAPLUS
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-bis(2-methylpropyl)- (CA INDEX NAME)

RN 913288-35-4 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl-N-methyl- (CA INDEX NAME)

RN 913288-36-5 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dipropyl- (CA INDEX NAME)

RN 913288-37-6 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-diethyl- (CA INDEX NAME)

RN 913288-38-7 HCAPLUS

CN Benzonitrile, 4-[[1-(1-piperidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-39-8 HCAPLUS

CN Benzonitrile, 4-[[1-(1-azetidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-40-1 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-propyl- (CA INDEX NAME)

RN 913288-41-2 HCAPLUS
CN Butanamide, N-butyl-N-(cyanomethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 913288-42-3 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(2-methoxyethyl)-N-propyl- (CA INDEX NAME)

$$CF_3$$
 N
 CH
 Et
 F_3C
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

RN 913288-43-4 HCAPLUS

CN Butanamide, N,N-bis(cyanomethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

$$CN$$
 CF_3
 N
 CH
 Et
 F_3C
 CH_2
 CH_2
 CH_2
 CH_2
 CH_3

RN 913288-44-5 HCAPLUS

CN Benzonitrile, 4-[[1-(4-morpholinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-45-6 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(cyclopropylmethyl)-N-propyl- (CA INDEX NAME)

RN 913288-46-7 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl-N-methyl- (CA INDEX NAME)

RN 913288-47-8 HCAPLUS

CN Benzonitrile, 4-[[1-(4-thiomorpholinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-48-9 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)

$$CF_3$$
 N
 CH
 Et
 F_3C
 CH_2
 C
 M
 M
 M
 M
 M

RN 913288-49-0 HCAPLUS

CN Butanamide, N-(2-cyanoethyl)-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 913288-50-3 HCAPLUS

CN Benzonitrile, 4-[[1-(1-pyrrolidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-51-4 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-(1-methylethyl)- (CA INDEX NAME)

RN 913288-52-5 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-di-2-propen-1-yl- (CA INDEX NAME)

RN 913288-53-6 HCAPLUS

CN Benzonitrile, 4-[[1-(3-thiazolidinylcarbonyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 913288-54-7 HCAPLUS

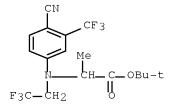
CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl-N-2-propen-1-yl- (CA INDEX NAME)

$$CF_3$$
 N
 CF_3
 N
 CH
 Et
 F_3C
 CH_2
 C
 N
 CH_2
 CH_2

RN 913288-58-1 HCAPLUS
CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]-N,N-dimethyl- (CA INDEX NAME)

IT 864283-58-9P 913288-72-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of N-cyanoaryl amino acid amides for treating endometriosis or
 uterine fibroids)
RN 864283-58-9 HCAPLUS
CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl) (CA INDEX NAME)

RN 913288-72-9 HCAPLUS
CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-,
1,1-dimethylethyl ester (CA INDEX NAME)



L41 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2005:1004698 HCAPLUS Full-text

DOCUMENT NUMBER: 143:286689

TITLE: Preparation of aniline amino acid derivatives as

selective androgen receptor modulators $% \left(1\right) =\left(1\right) \left(1\right)$

INVENTOR(S): Turnbull, Phillip Stewart; Cadilla,

Rodolfo; Cowan, David John;

Larkin, Andrew Lamont; Kaldor, Istvan

; Stewart, Eugene Lee

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 120 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PA:	CENT 1	NO.			KIND DATE			APPLICATION NO.						DATE					
	WO	√O 2005085185					_	20050915		WO 2005-US7245						20050303				
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,		
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,		
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,		
			SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,		
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,		
			MR,	ΝE,	SN,	TD,	ΤG													
	ΕP	P 1725522			A1 20061129			EP 2005-730067						20050303						
		R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,		
			IS,	ΙΤ,	LI,	LT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	HR,	LV		
	JP 2007526336						T 20070913				JP 2007-502061					20050303				
	US 20070191479						A1 20070816				US 2006-598508					20060901				
PRIOR	RIT	APP:	LN.	INFO	.:					US 2004-549794P						P 20040303				
	WO 2005-US7245												1	W 20050303						

OTHER SOURCE(S): CASREACT 143:286689; MARPAT 143:286689

ED Entered STN: 16 Sep 2005

AB The invention relates to non-steroidal compds. 3,4-R4R3C6H3NR1R2 [R1 is - (Q1)0-1-R5, where Q1 is alkylene and R5 is H, alkyl, alkenyl, alkynyl, haloalkyl or cycloalkyl; R2 is -Q3-Q4-R6 or -Q3-CN, where Q3 is alkylene, Q4is CO, CS, C:NR7, R7 is H or alkyl; R6 is alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryloxy or an amino group; R3 is CN, NO2 or halo; R4 is CN, NO2, halo, haloalkyl, alkyl, alkenyl, alkynyl, hydroxy, alkoxy, aryl or aryloxy] and their salts, solvates and physiol. functional derivs., that are modulators of

androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, as well as methods for their synthesis and use. Thus, N2-[4-cyano-3-(trifluoromethyl)phenyl]-N2-(cyclopropylmethyl)-N1- methylglycinamide wasprepared from 4-fluoro-2-(trifluoromethyl)benzonitrile by reaction with cyclopropylmethylamine and tert-Bu bromoacetate, followed by ester cleavage and methylamidation.

864283-35-2P 864283-36-3P 864283-46-5P ΙT 864283-47-6P 864283-48-7P 864283-57-8P 864283-58-9P 864283-59-0P 864283-68-1P 864283-71-6P 864284-22-0P 864284-40-2P 864284-52-6P 864284-55-9P 864284-74-2P 864284-76-4P 864284-84-4P 864284-95-7P 864285-03-0P 864285-13-2P 864285-15-4P 864285-17-6P 864285-25-6P 864285-37-0P 864285-45-0P 864285-47-2P 864285-55-2P 864285-57-4P 864285-65-4P 864285-67-6P 864285-69-8P 864285-77-8P 864285-79-0P 864285-85-8P 864285-87-0P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aniline amino acid derivs. as selective androgen receptor modulators)

RN 864283-35-2 HCAPLUS

Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)-, CN 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864283-36-3 HCAPLUS

Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA CN INDEX NAME)

864283-46-5 HCAPLUS RN

Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, CN 1,1-dimethylethyl ester (CA INDEX NAME)

$$CN$$
 CF_3
 N
 CH_2
 C
 CF_3
 C

RN 864283-47-6 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 864283-48-7 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864283-57-8 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, methyl ester (CA INDEX NAME)

RN 864283-58-9 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-(CA INDEX NAME)

RN 864283-59-0 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864283-68-1 HCAPLUS

CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864283-71-6 HCAPLUS

CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-22-0 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{Me} & \text{O} \\ \text{CH-C-OBu-t} \\ \text{CH}_2 - \text{N} \\ \text{CF}_3 \end{array}$$

RN 864284-40-2 HCAPLUS

CN Propanoic acid, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-2-methyl-, methyl ester (CA INDEX NAME)

RN 864284-52-6 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864284-55-9 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)

RN 864284-74-2 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864284-76-4 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 864284-84-4 HCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864284-95-7 HCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-03-0 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-13-2 HCAPLUS

CN Benzonitrile, 2-chloro-4-[(cyanomethyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

RN 864285-15-4 HCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O} \\ \text{CH-C-OBu-t} \\ & \text{CH}_2 - \text{N} \end{array}$$

RN 864285-17-6 HCAPLUS

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864285-25-6 HCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-37-0 HCAPLUS

CN Glycine, N-(3, 4-dicyanophenyl)-N-(2, 2, 2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-45-0 HCAPLUS

CN Alanine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-47-2 HCAPLUS CN Alanine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 864285-55-2 HCAPLUS

CN Butanoic acid, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-57-4 HCAPLUS

CN Butanoic acid, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864285-65-4 HCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-67-6 HCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)

RN 864285-69-8 HCAPLUS

CN Acetamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)

RN 864285-77-8 HCAPLUS

CN Alanine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-79-0 HCAPLUS

CN Alanine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{CN} \\ & \text{Ho}_2\text{C} & \text{CH} & \text{CN} \\ & \text{CH}_2 & \text{N} & \text{CN} \end{array}$$

RN 864285-85-8 HCAPLUS

CN Butanoic acid, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-87-0 HCAPLUS

CN Butanoic acid, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)

864283-37-4P 864283-38-5P 864283-49-8P ΙT 864283-50-1P 864283-51-2P 864283-52-3P 864283-53-4P 864283-54-5P 864283-55-6P 864283-56-7P 864283-60-3P 864283-62-5P 864283-65-8P 864283-74-9P 864283-77-2P 864283-80-7P 864283-83-0P 864284-16-2P 864284-19-5P 864284-25-3P 864284-27-5P 864284-29-7P 864284-31-1P 864284-33-3P 864284-35-5P 864284-37-7P 864284-42-4P 864284-48-0P 864284-50-4P 864284-57-1P 864284-59-3P 864284-62-8P 864284-78-6P 864284-80-0P 864284-82-2P 864284-87-7P 864284-89-9P 864284-91-3P 864284-93-5P 864284-97-9P 864284-99-1P 864285-01-8P 864285-05-2P 864285-07-4P 864285-09-6P 864285-11-0P 864285-19-8P 864285-21-2P 864285-23-4P 864285-27-8P 864285-29-0P 864285-31-4P 864285-33-6P 864285-35-8P 864285-39-2P 864285-41-6P 864285-43-8P

864285-49-4P 864285-51-8P 864285-53-0P 864285-59-6P 864285-61-0P 864285-63-2P 864285-71-2P 864285-73-4P 864285-75-6P 864285-81-4P 864285-83-6P 864285-89-2P 864285-91-6P 864285-93-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aniline amino acid derivs. as selective androgen receptor modulators)

RN 864283-37-4 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864283-38-5 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino](CA INDEX NAME)

RN 864283-49-8 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, methyl ester (CA INDEX NAME)

RN 864283-50-1 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1-methylethyl ester (CA INDEX NAME)

RN 864283-51-2 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864283-52-3 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864283-53-4 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-cyclohexyl- (CA INDEX NAME)

RN 864283-54-5 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

RN 864283-55-6 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1-methylhydrazide (CA INDEX NAME)

RN 864283-56-7 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 2,2-dimethylhydrazide (CA INDEX NAME)

RN 864283-60-3 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864283-62-5 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864283-65-8 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

RN 864283-74-9 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864283-77-2 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864283-80-7 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864283-83-0 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N,N-dimethyl- (CA INDEX NAME)

RN 864284-16-2 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864284-19-5 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864284-25-3 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864284-27-5 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]- (CA INDEX NAME)

RN 864284-29-7 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]-N-methyl- (CA INDEX NAME)

RN 864284-31-1 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]-N-ethyl- (CA INDEX NAME)

RN 864284-33-3 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]-N,N-dimethyl- (CA INDEX NAME)

RN 864284-35-5 HCAPLUS

CN Benzonitrile, 4-[(cyanomethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864284-37-7 HCAPLUS

CN Benzonitrile, 4-[(1-cyanoethy1)(2,2,2-trifluoroethy1)amino]-2-

(trifluoromethyl) - (CA INDEX NAME)

$$CN$$
 CF_3
 CN
 CH
 N
 CH
 Me

RN 864284-42-4 HCAPLUS

CN Benzonitrile, 4-[(2-cyanopropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864284-48-0 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoro-1-methylethyl)amino]- (CA INDEX NAME)

RN 864284-50-4 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl][1-(trifluoromethyl)propyl]amino]- (CA INDEX NAME)

RN 864284-57-1 HCAPLUS

CN Benzonitrile, 4-[(cyanomethyl)(3,3,3-trifluoropropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864284-59-3 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]- (CA INDEX NAME)

RN 864284-62-8 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](3,3,3-trifluoropropyl)amino]-N-methyl- (CA INDEX NAME)

RN 864284-78-6 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-80-0 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864284-82-2 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl-(CA INDEX NAME)

CN Alanine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 864284-89-9 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-91-3 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864284-93-5 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864284-97-9 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-99-1 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl- (CA INDEX NAME)

RN 864285-01-8 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864285-05-2 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864285-07-4 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

RN 864285-09-6 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-11-0 HCAPLUS

CN Acetamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-19-8 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

RN 864285-21-2 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-23-4 HCAPLUS

CN Propanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-27-8 HCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

RN 864285-29-0 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ \text{Et} & \text{CH} & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 864285-31-4 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-33-6 HCAPLUS

CN Butanamide, 2-[(3-chloro-4-cyanophenyl)(cyclopropylmethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-35-8 HCAPLUS

CN Glycine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)-, methyl ester (CA INDEX NAME)

RN 864285-39-2 HCAPLUS

CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864285-41-6 HCAPLUS

CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-43-8 HCAPLUS

CN Acetamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-49-4 HCAPLUS

CN Propanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864285-51-8 HCAPLUS

CN Propanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-53-0 HCAPLUS

CN Propanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-59-6 HCAPLUS

CN Butanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864285-61-0 HCAPLUS

CN Butanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-63-2 HCAPLUS

CN Butanamide, 2-[(3,4-dicyanophenyl)(2,2,2-trifluoroethyl)amino]-N-ethyl-(CA INDEX NAME)

RN 864285-71-2 HCAPLUS

CN Acetamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-methyl- (CA INDEX NAME)

RN 864285-73-4 HCAPLUS

CN Acetamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864285-75-6 HCAPLUS

CN 1,2-Benzenedicarbonitrile, 4-[(cyanomethyl)(cyclopropylmethyl)amino]- (CA INDEX NAME)

RN 864285-81-4 HCAPLUS

CN Propanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-methyl-(CA INDEX NAME)

RN 864285-83-6 HCAPLUS

CN Propanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-ethyl- (CA INDEX NAME)

RN 864285-89-2 HCAPLUS

CN Butanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 864285-91-6 HCAPLUS

CN Butanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-methyl- (CA INDEX NAME)

RN 864285-93-8 HCAPLUS

CN Butanamide, 2-[(cyclopropylmethyl)(3,4-dicyanophenyl)amino]-N-ethyl- (CA INDEX NAME)

IT 864286-08-8P 864286-10-2P 864286-12-4P

864286-19-1P 864286-21-5P 864286-23-7P

864286-27-1P 864286-29-3P 864286-31-7P

864286-34-0P 864286-36-2P 864286-38-4P

864286-55-5P 864286-61-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aniline amino acid derivs. as selective androgen receptor modulators)

RN 864286-08-8 HCAPLUS

CN 2-Propenoic acid, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, methyl ester (CA INDEX NAME)

RN 864286-10-2 HCAPLUS

CN Propanoic acid, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-2-methyl- (CA INDEX NAME)

RN 864286-12-4 HCAPLUS

CN Propanamide, 3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-2-methyl- (CA INDEX NAME)

RN 864286-19-1 HCAPLUS

CN Benzonitrile, 4-[2-propen-1-yl(2,2,2-trifluoro-1-methylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864286-21-5 HCAPLUS

CN Benzonitrile, 4-[(2-oxoethyl)(2,2,2-trifluoro-1-methylethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864286-23-7 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoro-1-methylethyl)- (CA INDEX NAME)

RN 864286-27-1 HCAPLUS

CN Benzonitrile, 4-[2-propen-1-yl[1-(trifluoromethyl)propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864286-29-3 HCAPLUS

CN Benzonitrile, 4-[(2-oxoethyl)[1-(trifluoromethyl)propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864286-31-7 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-[1-(trifluoromethyl)propyl]- (CA INDEX NAME)

RN 864286-34-0 HCAPLUS
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)(CA INDEX NAME)

RN 864286-36-2 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864286-38-4 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(3,3,3-trifluoropropyl)-(CA INDEX NAME)

RN 864286-55-5 HCAPLUS

CN Butanoic acid, 2-[(3-chloro-4-cyanophenyl)(2,2,2-trifluoroethyl)amino]-(CA INDEX NAME)

RN 864286-61-3 HCAPLUS

CN Glycine, N-(3,4-dicyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:1343064 HCAPLUS Full-text

DOCUMENT NUMBER: 146:287642

TITLE: Design and Synthesis of an Array of Selective Androgen

Receptor Modulators

AUTHOR(S): Trump, Ryan P.; Blanc, Jean-Baptiste E.; Stewart,

Hugene L.; Brown, Peter J.; Caivano, Matilde;

Gray, David W.; Hoekstra, William J.; Willson, Timothy

M.; Han, Bajin; Turnbull, Philip

CORPORATE SOURCE: GlaxoSmithKline, Research Triangle Park, NC, 27709,

USA

SOURCE: Journal of Combinatorial Chemistry (2007), 9(1),

107-114

CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 24 Dec 2006

AB We describe the design, using shape comparison and fast docking computer algorithms, and rapid parallel synthesis of a 1300 member array based on GSK7721, a 4-aminobenzonitrile androgen receptor (AR) antagonist identified by focused screening of the GSK compound collection. The array yielded 352 submicromolar and 17 subnanomolar AR agonists as measured by a cell-based

reporter gene functional assay. The rapid synthesis of a large number of active compds. provided valuable information in the optimization of AR modulators, which may be useful in treating androgen deficiency in aging males.

IT 821776-43-6P 821776-44-7P 821776-58-3P 927693-16-1P 927693-77-4P 927699-39-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Design and Synthesis of an Array of Selective Androgen Receptor Modulators)

RN 821776-43-6 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821776-44-7 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)

RN 821776-58-3 HCAPLUS

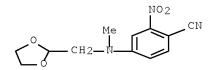
CN Benzonitrile, 2-chloro-4-[(cyclopropylmethyl)propylamino]- (CA INDEX NAME)

RN 927693-16-1 HCAPLUS

CN Benzonitrile, 2-chloro-4-[(1,3-dioxolan-2-ylmethyl)methylamino]- (CA INDEX NAME)

RN 927693-77-4 HCAPLUS

CN Benzonitrile, 4-[(1,3-dioxolan-2-ylmethyl)methylamino]-2-nitro- (CA INDEX NAME)



RN 927699-39-6 HCAPLUS

CN Benzonitrile, 4-[(1,3-dioxolan-2-ylmethyl)methylamino]- (CA INDEX NAME)

$$CH_2$$
 Me
 CN

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:1312622 HCAPLUS Full-text

DOCUMENT NUMBER: 146:62449

TITLE: Nonsteroidal tertiary arylamines as modulators of

androgen, glucocorticoid, mineralocorticoid, and progesterone receptors and their preparation and use

for treatment of diseases

Stewart, Eugene Lee; Stetson, Katherine

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 191pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006133216	A2	20061214	WO 2006-US21966	20060606
WO 2006133216	A3	20070426		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA EP 1888512 20080220 EP 2006-772327 20060606 Α2 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR PRIORITY APPLN. INFO.: US 2005-687895P P 20050606 WO 2006-US21966 W 20060606

OTHER SOURCE(S): MARPAT 146:62449

ED Entered STN: 15 Dec 2006

GΙ

This invention relates to non-steroidal compds. of formula I that are AΒ modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. Compds. of formula I wherein R1 is CN, NO2 and halo; n is 0, 1, and 2; each R3 is independently CN, NO2, halo, (halo)alkyl, alkenyl, alkynyl, OH, (halo)alkoxy, and aryl; R3 is (Rx)aR7; Rx is (un)substituted C1-4 alkylene; a is 0 and 1; R7 is H, (halo)alkyl, cycloalkyl, alkenyl, alkynyl, CN; R4 and R5 are independently H, (halo)alkyl, and cycloalkyl; R6 is (un)substituted aryl and (un) substituted heterocyclyl; and their pharmaceutically acceptable salts, and solvates thereof are claimed. Example compound II was prepared by substitution of 4-fluoro-2- trifluoromethylbenzonitrile with (R)-(+)-1-(2naphthyl)ethylamine; the resulting 4-[[(1R)-1-(2-naphthyl)ethyl]amino]-2trifluoromethylbenzonitrile underwent N-alkylation with cyclopropanemethyl bromide to give compound II. All the invention compds. were evaluated for their androgen, glucocorticoid, mineralocorticoid, and progesterone receptor modulatory activity. From the assay, it was determined that some of the compds. exhibited pIC50 values of \geq 5.0.

IT 916807-89-1P 916808-25-8P 916808-26-9P 916808-52-1P 916808-53-2P 916808-58-7P 916808-60-1P 916808-67-8P 916808-71-4P 916809-17-1P 916809-19-3P 916809-37-5P 916809-38-6P 916809-83-1P 916809-89-7P 916809-99-9P 916810-00-9P 916810-05-4P

916810-24-7P 916810-35-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate and intermediate; preparation of nonsteroidal tertiary arylamines as modulators of androgen, glucocorticoid, mineralocorticoid and progesterone receptors useful in therapy)

RN 916807-89-1 HCAPLUS

CN Benzonitrile, 4-[[(3-bromophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Br} \\ \text{F}_3\text{C} - \text{CH}_2 \\ \text{CH}_2 - \text{N} \end{array}$$

RN 916808-25-8 HCAPLUS

CN 2-Furancarboxylic acid, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, ethyl ester (CA INDEX NAME)

RN 916808-26-9 HCAPLUS

CN 2-Furancarboxamide, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-52-1 HCAPLUS

CN 3-Furancarboxylic acid, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{F}_{3}\text{C-}_{\text{CH}_{2}} \\ \text{CH}_{2} \\ \text{C-}_{\text{OMe}} \end{array}$$

RN 916808-53-2 HCAPLUS

CN 3-Furancarboxamide, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-58-7 HCAPLUS

CN Benzonitrile, 4-[[(5-chloro-2-thienyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$C1$$
 S
 CH_2
 CH_3
 CN
 CH_2
 CH_3
 CN

RN 916808-60-1 HCAPLUS

CN Benzonitrile, 4-[[(5-bromo-2-thienyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-67-8 HCAPLUS

CN 1H-Imidazole-1-carboxylic acid, 4-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 916808-71-4 HCAPLUS

CN Benzonitrile, 4-[[[4-(hydroxymethyl)-2-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

HO—
$$CH_2$$
 N
 CH_2
 CF_3
 CN

RN 916809-17-1 HCAPLUS

CN Carbamic acid, N-[[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]methyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

RN 916809-19-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(aminomethyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-37-5 HCAPLUS

CN 1-Piperidinecarboxylic acid, 3-[3-[[[4-cyano-3-

(trifluoromethyl) phenyl] (2, 2, 2-trifluoroethyl) amino]methyl]-1, 2, 4-oxadiazol-5-yl]-, 1, 1-dimethylethyl ester (CA INDEX NAME)

RN 916809-38-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-piperidinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-83-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(5-bromo-3-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-89-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-99-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-nitrophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-00-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-aminophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-05-4 HCAPLUS

CN Benzonitrile, 4-[[[5-[4-(methylthio)phenyl]-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-24-7 HCAPLUS

CN Benzonitrile, 4-[[(4,5-dihydro-5-oxo-1,3,4-oxadiazol-2-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ \text{CH2} \\ \text{CH2} \\ \end{array}$$

RN 916810-35-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-4-(phenylmethyl)-4H-1,2,4-triazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} F & CH_2 - Ph \\ \hline N & F_3C - CH_2 \\ \hline N - N & CH_2 - N \end{array} \xrightarrow{CF3} CN$$

916807-39-1P 916807-59-5P 916807-71-1P ΙT 916807-75-5P 916807-78-8P 916807-81-3P 916807-83-5P 916807-86-8P 916807-87-9P 916807-88-0P 916807-90-4P 916807-91-5P 916807-92-6P 916807-93-7P 916807-95-9P 916807-96-0P 916807-97-1P 916807-98-2P 916807-99-3P 916808-00-9P 916808-01-0P 916808-02-1P 916808-03-2P 916808-04-3P 916808-05-4P 916808-06-5P 916808-07-6P 916808-08-7P 916808-09-8P 916808-10-1P 916808-11-2P 916808-12-3P 916808-13-4P 916808-14-5P 916808-15-6P 916808-16-7P 916808-17-8P 916808-18-9P 916808-19-0P 916808-20-3P 916808-21-4P 916808-22-5P 916808-23-6P 916808-24-7P 916808-27-0P 916808-28-1P 916808-29-2P 916808-30-5P

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916810-31-6P 916810-32-7P 916810-33-8P
916810-34-9P 916810-36-1P 916810-37-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
```

(drug candidate; preparation of nonsteroidal tertiary arylamines as modulators of androgen, glucocorticoid, mineralocorticoid and progesterone receptors useful in therapy)

RN 916807-39-1 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[(1R)-1-(2-naphthalenyl)ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 916807-59-5 HCAPLUS

CN Benzonitrile, 4-[(1-cyclopropylethyl)(phenylmethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-71-1 HCAPLUS

CN Benzonitrile, 4-[(phenylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-75-5 HCAPLUS

CN Benzonitrile, 4-[[(2-methylphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-78-8 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[2-(trifluoromethyl)phenyl]methyl] amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-81-3 HCAPLUS

CN Benzonitrile, 4-[[(2-fluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-83-5 HCAPLUS

CN Benzonitrile, 4-[[(3-methylphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-86-8 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-(trifluoromethyl)phenyl]methyl] amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-87-9 HCAPLUS

CN Benzonitrile, 4-[[(3-fluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-88-0 HCAPLUS

CN Benzonitrile, 4-[[(3-chlorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-90-4 HCAPLUS

CN Benzonitrile, 4-[([1,1'-biphenyl]-3-ylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-91-5 HCAPLUS

CN Benzonitrile, 4-[[(3-methoxyphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-92-6 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-(trifluoromethoxy)phenyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-93-7 HCAPLUS

CN Benzonitrile, 4-[[[3-(4-fluorophenoxy)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-95-9 HCAPLUS

CN Benzonitrile, 4-[[[3-(2-fluorophenoxy)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-96-0 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-[(trifluoromethyl)thio]phenyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-97-1 HCAPLUS

CN Benzonitrile, 4-[[(3-cyanophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916807-98-2 HCAPLUS

CN Benzoic acid, 3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, methyl ester (CA INDEX NAME)

$$F_3C-CH_2$$

$$CH_2-N$$

$$CH_2-N$$

RN 916807-99-3 HCAPLUS

CN Benzamide, 3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

$$F_3C-CH_2$$
 CH_2
 CH

RN 916808-00-9 HCAPLUS

CN Benzonitrile, 4-[[(3-nitrophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-01-0 HCAPLUS

CN Benzonitrile, 4-[[(4-methylphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-02-1 HCAPLUS

CN Benzonitrile, 4-[[[4-(1,1-dimethylethyl)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-03-2 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[4-(trifluoromethyl)phenyl]methyl] amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-04-3 HCAPLUS

CN Benzonitrile, 4-[[(4-fluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-05-4 HCAPLUS

CN Benzonitrile, 4-[[(4-methoxyphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-06-5 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[4-(trifluoromethoxy)phenyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-07-6 HCAPLUS

CN Benzonitrile, 4-[[[4-(methylsulfonyl)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-08-7 HCAPLUS

CN Benzonitrile, 4-[[(4-cyanophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-09-8 HCAPLUS

CN Benzoic acid, 4-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} - \overset{\bigcirc}{\text{U}} \\ \\ \text{CH}_2 - \overset{\bigcirc}{\text{N}} \\ \end{array}$$

RN 916808-10-1 HCAPLUS

CN Benzonitrile, 4-[[(4-nitrophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-11-2 HCAPLUS

CN Benzonitrile, 4-[[(3,5-dimethylphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-12-3 HCAPLUS

CN Benzonitrile, 4-[[[3,5-bis(trifluoromethyl)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-13-4 HCAPLUS

CN Benzonitrile, 4-[[(3,5-dimethoxyphenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-14-5 HCAPLUS

CN Benzonitrile, 4-[[(3,5-dichlorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-15-6 HCAPLUS

CN Benzonitrile, 4-[[(3,5-difluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-16-7 HCAPLUS

CN Benzonitrile, 4-[[(2,6-difluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-17-8 HCAPLUS

CN Benzonitrile, 4-[[(2,4-difluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-18-9 HCAPLUS

CN Benzonitrile, 4-[[(3,4-difluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-19-0 HCAPLUS

CN Benzonitrile, 4-[[(2,3-difluorophenyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-20-3 HCAPLUS

CN Benzonitrile, 4-[[[3-fluoro-4-(trifluoromethyl)phenyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_{3}C - CH_{2} \qquad F_{3}C - CH_{2}$$

RN 916808-21-4 HCAPLUS

CN Benzonitrile, 4-[(2-naphthalenylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-22-5 HCAPLUS

CN Benzonitrile, 4-[(1-phenylethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-23-6 HCAPLUS

CN Benzonitrile, 4-[(3-furanylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-24-7 HCAPLUS

CN Benzonitrile, 4-[(2-furanylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-27-0 HCAPLUS

CN 2-Furancarbonitrile, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-28-1 HCAPLUS

CN Benzonitrile, 4-[[(5-methyl-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-29-2 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-(trifluoromethyl)-2-furanyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-30-5 HCAPLUS

CN 2-Furanacetonitrile, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

$$NC = CH_2$$
 O
 $CH_2 = CH_2$
 CH_3
 CN

RN 916808-31-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(methoxymethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$MeO=CH_2 O CH_2 O CH_2 N$$

RN 916808-32-7 HCAPLUS

CN Benzonitrile, 4-[[[5-[(2,2,2-trifluoroethoxy)methyl]-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-33-8 HCAPLUS

CN Benzonitrile, 4-[[[5-[(methylthio)methyl]-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$MeS = CH_2$$

$$CH_2$$

$$CH_2$$

$$CH_2$$

$$CH_3$$

$$CN$$

RN 916808-34-9 HCAPLUS

CN Benzonitrile, 4-[[[5-[(dimethylamino)methyl]-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-35-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(1H-imidazol-1-ylmethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$NC$$
 $CF3$
 CH_2-CF_3
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

RN 916808-36-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(1H-1,2,4-triazol-1-ylmethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-37-2 HCAPLUS

CN 2-Furanpropanenitrile, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

$$\text{NC}$$
 CH_2 $\text{CH}_$

RN 916808-38-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,5-difluorophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-39-4 HCAPLUS

CN Benzonitrile, 4-[[(5-phenyl-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2 CF_3$$

$$CH_2 - N$$

RN 916808-40-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-41-8 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,4-difluorophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-42-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(2,4-difluorophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-43-0 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[4-(trifluoromethoxy)phenyl]-2-furanyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-44-1 HCAPLUS

CN Acetamide, N-[4-[5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-2-furanyl]phenyl]- (CA INDEX NAME)

RN 916808-45-2 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-cyanophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-46-3 HCAPLUS

CN Benzonitrile, 4-[[[5-[4-(methylsulfonyl)phenyl]-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$Me - \bigcup_{0}^{\circ} \bigcup_{CH_{2} - N}^{CF_{3}} \bigcup_{CH_{2} - N}^{CF_{3}} \bigcup_{CN_{2} - N$$

RN 916808-47-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-cyanophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-48-5 HCAPLUS

CN 2-Thiophenecarbonitrile, 5-[5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-2-furanyl]- (CA INDEX NAME)

$$NC$$
 CF_3
 CH_2-CF_3
 CH_2
 CH_2
 CH_3
 CH_2
 CH_3
 CH_3

RN 916808-49-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(5-pyrimidinyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-50-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,5-dimethyl-4-isoxazolyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-51-0 HCAPLUS

CN Benzonitrile, 4-[[[4-(4-cyanophenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-54-3 HCAPLUS

CN 3-Furancarbonitrile, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-55-4 HCAPLUS

CN Benzonitrile, 4-[[[3-(hydroxymethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-56-5 HCAPLUS

CN Benzonitrile, 4-[[(3-methyl-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-57-6 HCAPLUS

CN Benzonitrile, 4-[(2-benzofuranylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-59-8 HCAPLUS

CN Benzonitrile, 4-[(2-thienylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-61-2 HCAPLUS

CN 2-Thiophenecarbonitrile, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-62-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-2-thienyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-63-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-cyanophenyl)-2-thienyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-64-5 HCAPLUS

CN Benzonitrile, 4-[(3-thienylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CH_2$$
 $N-CH_2-CF_3$
 F_3C

RN 916808-65-6 HCAPLUS

CN Benzonitrile, 4-[[(5-chlorobenzo[b]thien-3-y1)methy1](2,2,2-trifluoroethy1)amino]-2-(trifluoromethy1)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \text{CF3} \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 916808-66-7 HCAPLUS

CN Benzonitrile, 4-[(1H-imidazol-2-ylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-68-9 HCAPLUS

CN Benzonitrile, 4-[(1H-imidazol-5-ylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-69-0 HCAPLUS

CN Benzonitrile, 4-[(2-oxazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-70-3 HCAPLUS

CN Benzonitrile, 4-[(4-oxazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C-CH_2$$

$$CH_2-N$$

$$CH_2-N$$

RN 916808-72-5 HCAPLUS

CN 4-Oxazolecarbonitrile, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-73-6 HCAPLUS

CN 5-Oxazolecarbonitrile, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-74-7 HCAPLUS

CN Benzonitrile, 4-[[[5-[(phenylmethoxy)methyl]-2-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-75-8 HCAPLUS

CN Benzonitrile, 4-[[[2-(4-fluorophenyl)-4-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-76-9 HCAPLUS

CN Benzonitrile, 4-[[(4-phenyl-2-oxazolyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-77-0 HCAPLUS

CN 2-Oxazolecarbonitrile, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916808-78-1 HCAPLUS

CN Benzonitrile, 4-[[[2-(4-fluorophenyl)-5-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-79-2 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-2-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-80-5 HCAPLUS

CN Benzonitrile, 4-[(5-oxazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-81-6 HCAPLUS

CN Benzonitrile, 4-[[(3,5-dimethyl-4-isoxazolyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$Me$$
 CH_2
 $M-CH_2-CF_3$
 F_3C

RN 916808-82-7 HCAPLUS

CN Benzonitrile, 4-[[(5-methyl-3-isoxazolyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-83-8 HCAPLUS

CN Benzonitrile, 4-[(5-isoxazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-84-9 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(4-thiazolylmethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2
 CH_3
 CH_3

RN 916808-85-0 HCAPLUS

CN Benzonitrile, 4-[(4-thiazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C-CH_2$$
 CH_2
 CH_2
 CH_2
 CH_3
 CH

CN Benzonitrile, 4-[[(2-methyl-4-thiazolyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CF 3} \\ \text{F 3C-CH2} \\ \text{CH2-N} \end{array}$$

RN 916808-87-2 HCAPLUS

CN Benzonitrile, 4-[[(2-phenyl-4-thiazolyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-88-3 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[2-[4-(trifluoromethyl)phenyl]-4-thiazolyl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-89-4 HCAPLUS

CN Benzonitrile, 4-[[[2-(2-thienyl)-4-thiazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-90-7 HCAPLUS

CN Benzonitrile, 4-[(2-benzothiazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-91-8 HCAPLUS

CN Benzonitrile, 4-[(5-thiazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 916808-92-9 HCAPLUS

CN Benzonitrile, 4-[(2-thiazolylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-93-0 HCAPLUS

CN Benzonitrile, 4-[[1-(2-thiazolyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\stackrel{\text{Me}}{\underset{S}{\longleftarrow}} CH = N - R$$

RN 916808-94-1 HCAPLUS

CN Benzonitrile, 2-chloro-4-[(4-thiazolylmethyl)(2,2,2-trifluoroethyl)amino]-(CA INDEX NAME)

RN 916808-95-2 HCAPLUS

CN 1,2-Benzenedicarbonitrile, 4-[(cyclopropylmethyl)(4-thiazolylmethyl)amino]-(CA INDEX NAME)

RN 916808-96-3 HCAPLUS

CN 1,2-Benzenedicarbonitrile, 4-[(4-thiazolylmethyl)(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 916808-97-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(1,1-dimethylethyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX

NAME)

RN 916808-98-5 HCAPLUS

CN Benzonitrile, 4-[[(5-phenyl-1,2,4-oxadiazol-3-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916808-99-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-methoxyphenyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-00-2 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-01-3 HCAPLUS

CN 1-Piperidinesulfonamide, 4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-)]

trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]- (CA INDEX NAME)

RN 916809-02-4 HCAPLUS

CN Benzonitrile, 4-[(1,2,4-oxadiazol-3-ylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-03-5 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-methylethyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-04-6 HCAPLUS

CN Benzonitrile, 4-[[(5-methyl-1,2,4-oxadiazol-3-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-05-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-methylpropyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-1)

trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-06-8 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2 - CH_2$$

$$CH_2 - N$$

$$F_3C$$

RN 916809-07-9 HCAPLUS

CN Benzonitrile, 4-[[(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-08-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-09-1 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)][[5-[4-(trifluoromethoxy)phenyl]-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-10-4 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)][[5-[4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

F3C
$$CH_2$$
 CH_2 $CH_$

RN 916809-11-5 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[3-(trifluoromethoxy)phenyl]-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-12-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(5-isoxazolyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$NC$$
 $CF3$
 $CH2-CF3$
 $N-CH2$
 N

RN 916809-13-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-thienyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-

trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-15-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,5-dimethyl-4-isoxazolyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-20-6 HCAPLUS

CN Acetamide, N-[[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} & & \text{CF}_3 \\ & & \text{CH}_2 - \text{N} \end{array}$$

RN 916809-21-7 HCAPLUS

CN Methanesulfonamide, N-[[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]methyl]- (CA INDEX NAME)

RN 916809-22-8 HCAPLUS

CN Urea, N-[[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]methyl]- (CA INDEX NAME)

RN 916809-23-9 HCAPLUS

CN Urea, N-(aminocarbonyl)-N'-[[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]methyl]- (CA INDEX NAME)

RN 916809-24-0 HCAPLUS

CN Carbamic acid, N-[2-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 916809-25-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-aminoethyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2$$

$$CH_2 - CH_2$$

$$H_2N - CH_2 - CH_2$$

RN 916809-26-2 HCAPLUS

CN Acetamide, N-[2-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]ethyl]- (CA INDEX NAME)

RN 916809-27-3 HCAPLUS

CN Methanesulfonamide, N-[2-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]ethyl]- (CA INDEX NAME)

$$\begin{array}{c} & & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & \\ & & \\ & \\ & \\ & & \\ & \\ & & \\ & \\ & \\ & & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ &$$

RN 916809-28-4 HCAPLUS

CN Urea, N-[2-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]ethyl]- (CA INDEX NAME)

RN 916809-29-5 HCAPLUS

CN Urea, N-(aminocarbonyl)-N'-[2-[3-[[[4-cyano-3-

(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4oxadiazol-5-yl]ethyl]- (CA INDEX NAME)

RN 916809-30-8 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-acetyl-4-piperidinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-31-9 HCAPLUS

CN Benzonitrile, 4-[[[5-[1-(5-isoxazolylcarbonyl)-4-piperidinyl]-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-(CA INDEX NAME)

RN 916809-32-0 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{CH}_2 \\ \\ \text{N} \end{array} \begin{array}{c} \text{CF3} \\ \\ \text{CN} \\ \\ \text{CH}_2 \\ \\ \text{N} \end{array}$$

RN 916809-33-1 HCAPLUS

CN 1-Piperidinecarboxamide, 4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]- (CA INDEX NAME)

$$H_2N$$
 N
 CF_3
 CH_2
 N
 CH_2
 N
 CH_2
 N
 CH_3
 CN

RN 916809-34-2 HCAPLUS

CN 1-Piperidinecarboxamide, 4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-N-methyl- (CA INDEX NAME)

RN 916809-35-3 HCAPLUS

CN Benzonitrile, 4-[[[5-[1-(methylsulfonyl)-4-piperidinyl]-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-36-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-methyl-4-piperidinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

Me
$$_{N}$$
 $_{CH_{2}}$ $_{CH_{2}}$ $_{CH_{2}}$ $_{CH_{3}}$ $_{CN}$

RN 916809-39-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-acetyl-3-piperidinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-40-0 HCAPLUS

CN 1-Piperidinecarboxylic acid, 3-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-, methyl ester (CA INDEX NAME)

RN 916809-41-1 HCAPLUS

CN 1-Piperidinecarboxamide, 3-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]- (CA INDEX NAME)

RN 916809-42-2 HCAPLUS

CN 1-Piperidinecarboxamide, 3-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-N-methyl- (CA INDEX NAME)

RN 916809-43-3 HCAPLUS

CN Benzonitrile, 4-[[[5-[1-(methylsulfonyl)-3-piperidinyl]-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-44-4 HCAPLUS

CN Benzonitrile, 4-[[(5-benzoyl-1,2,4-oxadiazol-3-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-46-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-furanylcarbonyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

CN Benzonitrile, 4-[[[5-(2-pyridinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{CF3} \\
 & \text{CH}_2 \\
 & \text{N}
\end{array}$$

RN 916809-51-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(cyclopropylmethyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$NC$$
 $CF3$
 CH_2-CF_3
 $N-CH_2$
 CH_2
 CH_2
 CH_2

RN 916809-53-5 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-(2,2,2-trifluoroethyl)-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-54-6 HCAPLUS

CN Benzonitrile, 4-[[[5-[(dimethylamino)methyl]-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-57-9 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[6-(trifluoromethyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-60-4 HCAPLUS

CN Benzonitrile, 4-[[[3-(4-fluorophenyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_{3}C-CH_{2}$$

$$CH_{2}-N$$

$$CH_{2}-N$$

RN 916809-63-7 HCAPLUS

CN Benzonitrile, 4-[[[3-(2-pyridinyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-65-9 HCAPLUS

CN Benzonitrile, 4-[[(3-phenyl-1,2,4-oxadiazol-5-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ \text{F3C-CH2} \\ \text{CH2-N} \end{array}$$

RN 916809-68-2 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-[4-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-71-7 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-[4-(trifluoromethoxy)phenyl]-1,2,4-oxadiazol-5-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

F3C-O

$$\begin{array}{c}
F_3C-CH_2 \\
CH_2-N
\end{array}$$
 $\begin{array}{c}
CF_3 \\
CN
\end{array}$

RN 916809-72-8 HCAPLUS

CN Benzonitrile, 4-[[[3-[4-(1,1-dimethylethyl)phenyl]-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-73-9 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

CN Benzonitrile, 4-[[[3-(3-pyridinyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-75-1 HCAPLUS

CN Benzonitrile, 4-[[[3-[3,5-bis(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CF3} & \text{F3C-CH2} \\ \text{F3C} & \text{CH2-N} \end{array}$$

RN 916809-76-2 HCAPLUS

CN Benzonitrile, 4-[[[3-(3-nitrophenyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-77-3 HCAPLUS

CN Benzonitrile, 4-[[[3-[[(4-fluorophenyl)sulfonyl]methyl]-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-78-4 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[3-[6-(trifluoromethyl)-3-pyridinyl]-1,2,4-oxadiazol-5-yl]methyl]amino]-2-(trifluoromethyl)- (CA

INDEX NAME)

F3C
$$CH_2$$
 CH_2 $CH_$

RN 916809-79-5 HCAPLUS

CN Benzonitrile, 4-[[[3-(2,4-dichlorophenyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-80-8 HCAPLUS

CN Benzonitrile, 4-[[[3-(2,3-dichlorophenyl)-1,2,4-oxadiazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-81-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-methylphenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-82-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-84-2 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-chloro-4-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C-CH_2$$

$$CH_2-N$$

$$CH_2-N$$

$$CH_2-N$$

RN 916809-85-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(6-chloro-3-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-86-4 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)][[5-[6-(trifluoromethyl)-3-

pyridinyl]-1,3,4-oxadiazol-2-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-87-5 HCAPLUS

CN Benzonitrile, 4-[[[5-(6-chloro-2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-88-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(6-fluoro-2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-90-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-methylphenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-91-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-92-2 HCAPLUS

CN Benzonitrile, 4-[[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-93-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-94-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-furanyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 916809-95-5 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-96-6 HCAPLUS

CN Benzonitrile, 4-[[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-97-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(1,3-benzodioxol-5-yl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916809-98-8 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-thienyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} N \\ CH_2 \\ N - CH_2 - CF_3 \end{array}$$

RN 916810-01-0 HCAPLUS

CN Acetamide, N-[4-[5-[[[4-cyano-3-(trifluoromethyl)phenyl]](2,2,2-trifluoroethyl)amino]methyl]-1,3,4-oxadiazol-2-yl]phenyl]- (CA INDEX NAME)

RN 916810-02-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-methylphenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2 -$$

RN 916810-03-2 HCAPLUS

CN Benzonitrile, 4-[[[5-(3-fluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-04-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-06-5 HCAPLUS

CN Benzonitrile, 4-[[[5-[4-(methylsulfinyl)phenyl]-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-07-6 HCAPLUS

CN Benzonitrile, 4-[[[5-[4-(methylsulfonyl)phenyl]-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

F3C-CH2 CN

$$CF_3$$
 CH_2
 CH_2

RN 916810-08-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(5-bromo-2-furanyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C$$

$$CH_2$$

$$N-CH_2-CF_3$$

$$CN$$

RN 916810-09-8 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[4-(trifluoromethoxy)phenyl]-1,3,4-oxadiazol-2-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-10-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,4-difluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2$$

$$CH_2 - N$$

$$F_3C - CH_2$$

$$CH_3 - CN$$

$$CH_2 - N$$

RN 916810-11-2 HCAPLUS

CN Carbamic acid, N-[[5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,3,4-oxadiazol-2-yl]methyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

$$F_3C - CH_2$$

$$CH_2 - N$$

$$CH_2 - N$$

$$CH_2 - N$$

RN 916810-12-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(3,5-difluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C = CH_2$$

$$CH_2 = N$$

$$F_3C = CH_2$$

$$CH_2 = N$$

RN 916810-13-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(6-bromo-2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-14-5 HCAPLUS

CN Benzonitrile, 4-[[[5-(2,4-difluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-15-6 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[2-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C$$
— CH_2 — CH_3 — CH_2 — CH_3 —

RN 916810-16-7 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[3-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-17-8 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-fluorophenyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-18-9 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[[5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]methyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-19-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-chloro-6-methoxy-4-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-20-3 HCAPLUS

CN Benzonitrile, 4-[[[5-(1,3-dimethyl-1H-pyrazol-5-yl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{CH2} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CN} \\ \text{CN} \end{array}$$

RN 916810-21-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-pyrazinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-22-5 HCAPLUS

CN Benzonitrile, 4-[[[5-(5-pyrimidinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-23-6 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-methyl-1H-pyrazol-3-yl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-25-8 HCAPLUS

CN Benzonitrile, 4-[[(4,5-dihydro-4-methyl-5-oxo-1,3,4-oxadiazol-2-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-26-9 HCAPLUS

CN Benzonitrile, 4-[[[5-(dimethylamino)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2$$

$$CH_2 - N$$

$$Me 2N$$

$$CH_2 - N$$

RN 916810-27-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-morpholinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-28-1 HCAPLUS

CN Benzonitrile, 4-[[[5-(1-piperidinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-29-2 HCAPLUS

CN Benzonitrile, 4-[[(5-amino-1,3,4-oxadiazol-2-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2$$
 CF_3
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_3
 CH_3

RN 916810-30-5 HCAPLUS

CN Benzonitrile, 2-chloro-4-[(cyclopropylmethyl)[[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl]amino]- (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2

RN 916810-31-6 HCAPLUS

CN Benzonitrile, 2-chloro-4-[[[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 916810-32-7 HCAPLUS

CN 1,2-Benzenedicarbonitrile, 4-[(cyclopropylmethyl)[[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl]amino]- (CA INDEX NAME)

RN 916810-33-8 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-pyridinyl)-1H-1,2,4-triazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-34-9 HCAPLUS

CN Benzonitrile, 4-[[[3-(5-bromo-3-pyridinyl)-1H-1,2,4-triazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \text{CF3} \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 916810-36-1 HCAPLUS

CN Benzonitrile, 4-[[[3-(4-fluorophenyl)-1H-1,2,4-triazol-5-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-37-2 HCAPLUS

CN Benzonitrile, 4-[[(2-methyl-2H-tetrazol-5-yl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CF3} \\ \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \end{array}$$

IT 864283-46-5P 864283-47-6P 864283-48-7P 864284-35-5P 864284-74-2P 864284-76-4P 864285-03-0P 864285-05-2P 864285-65-4P 864285-67-6P 916810-42-9P 916810-43-0P 916810-44-1P 916810-45-2P 916810-46-3P 916810-47-4P 916810-48-5P 916810-49-6P 916810-50-9P 916810-53-2P 916810-58-7P

916810-72-5P 916810-73-6P 916810-74-7P

916810-75-8P 916810-76-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of nonsteroidal tertiary arylamines as modulators

of androgen, glucocorticoid, mineralocorticoid and progesterone receptors useful in therapy)

RN 864283-46-5 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864283-47-6 HCAPLUS
CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)(CA INDEX NAME)

RN 864283-48-7 HCAPLUS
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-35-5 HCAPLUS
CN Benzonitrile, 4-[(cyanomethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864284-74-2 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864284-76-4 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(2,2,2-trifluoroethyl)- (CA INDEX NAME)

RN 864285-03-0 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-05-2 HCAPLUS

CN Glycine, N-(3-chloro-4-cyanophenyl)-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864285-65-4 HCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 864285-67-6 HCAPLUS

CN Glycine, N-(cyclopropylmethyl)-N-(3,4-dicyanophenyl)- (CA INDEX NAME)

RN 916810-42-9 HCAPLUS

CN 2-Furancarboxylic acid, 5-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]- (CA INDEX NAME)

RN 916810-43-0 HCAPLUS

CN Benzonitrile, 4-[[[5-(hydroxymethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-44-1 HCAPLUS

CN Benzonitrile, 4-[[[5-[(acetyloxy)methyl]-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-45-2 HCAPLUS

CN Benzonitrile, 4-[[[5-(chloromethyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$C1CH_2$$
 O CH_2 CH_2 CH_3 CN

RN 916810-46-3 HCAPLUS

CN Benzonitrile, 4-[[(5-formyl-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-47-4 HCAPLUS

CN Benzonitrile, 4-[[[5-(2-cyanoethenyl)-2-furanyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-48-5 HCAPLUS

CN Benzonitrile, 4-[[(5-bromo-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-49-6 HCAPLUS

CN Benzonitrile, 4-[[(4-bromo-2-furanyl)methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-50-9 HCAPLUS

CN Benzonitrile, 4-[[[1-(phenylmethyl)-1H-imidazol-2-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-53-2 HCAPLUS

CN 4-Oxazolecarboxylic acid, 2-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-, methyl ester (CA INDEX NAME)

RN 916810-58-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(hydroxymethyl)-2-oxazolyl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C - CH_2$$

$$CH_2 - N$$

$$CH_2 - N$$

$$CH_2 - N$$

RN 916810-72-5 HCAPLUS

CN Ethanimidamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-hydroxy- (CA INDEX NAME)

RN 916810-73-6 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 916810-74-7 HCAPLUS

CN Benzonitrile, 4-[[[5-(4-piperidinyl)-1,2,4-oxadiazol-3-yl]methyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 916810-75-8 HCAPLUS

CN Carbamic acid, N-[[4-[3-[[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]methyl]-1,2,4-oxadiazol-5-yl]-1-piperidinyl]sulfonyl]-

, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 916810-76-9 HCAPLUS

CN Acetic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-, hydrazide (CA INDEX NAME)

IT 916810-77-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of nonsteroidal tertiary arylamines as
modulators of androgen, glucocorticoid, mineralocorticoid and
progesterone receptors useful in therapy)

RN 916810-77-0 HCAPLUS

CN Benzonitrile, 4-[(2H-tetrazol-5-ylmethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{F3C-CH2} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{H} \end{array}$$

L41 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:383697 HCAPLUS Full-text

DOCUMENT NUMBER: 144:432552

TITLE: Preparation of substituted anilines as selective

androgen receptor modulators
INVENTOR(S): Turnbull, Philip Stewart; Larkin,

Andrew Lamont; Kaldor, Istvan; Cadilla, Rodolfo; Cowan, David John;

Stewart, Eugene Lee

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 134 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GΙ

	PATENT NO.					KIND		DATE		APPLICATION NO.					DATE				
	WO	0 2006044707				A1 20060			0427	27 WO 2005-US37094						20051013			
		W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KP,	KR,	KΖ,	
			LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	
			NA,	NG,	NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	
			SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	
			YU,	ZA,	ZM,	ZW													
		RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	
			IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
			CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,	GH,	
			GM,	KΕ,	LS,	MW,	MΖ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
			KG,	KΖ,	MD,	RU,	ТJ,	$_{ m MT}$											
	EP 1809275				A1 20070725				EP 2005-812180						20051013				
		R:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	
			IS,	ΙT,	LI,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	HR	
	JP 2008515998						20080515 JP 2007-536962 200								0051	013			
PRIO	PRIORITY APPLN. INFO.:									US 2004-618480P					P 20041013				
												WO 2005-US37094							
OTHER SOURCE(S): CASREACT 144:432552; MARPAT 144:432552																			
ED	Ent	cered	STN	: 2	7 Ap:	r 20	06												

$$R^{2}m$$
 R^{3}
 R^{4}
 R^{5}
 $R^{6}n$
 R^{3}
 $R^{6}n$
 $R^{6}n$
 $R^{6}n$

This invention relates to non-steroidal compds. I [R1 = CN or NO2; R2 = independently CN, NO2, halo, etc.; R3 = H, (cyclo)alkyl, alkoxycarbonylalkyl, etc.; R4, R5 = independently H, (cyclo)alkyl, halo, etc., or R4R5 = (un)substituted (hetero)cyclyl; Y = (un)substituted methylene(oxy), methylenethio, carbonylamino, etc.; A = (hetero)aryl or heterocyclyl; m = 0-2; n = 0-5; R6 = independently (halo)alkyl, halo, hydroxy, etc.] which are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. For example, II was provided in a multi-step synthesis starting from the reaction of 4-fluoro-2-(trifluoromethyl)benzonitrile with 1-

cyclopropylmethanamine. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given).

ΙT 884854-00-6P, 1,1-Dimethylethyl [4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]phenyl]carba mate 884854-06-2P, Methyl 4-[[2-[[4-cyano-3-(trifluoromethy1)pheny1](2,2,2-trifluoroethy1)amino]ethy1]oxy]benzoate 884854-97-3P, 4-[[2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2trifluoroethyl)amino]ethyl]oxy]benzoic acid 884854-14-2P, 4-[[2-[[4-(Trifluoroacetyl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-57-3P, 4-[[2-(Phenylthio) ethyl] (2,2,2-trifluoroethyl) amino]-2-(trifluoromethyl)benzonitrile 884854 - 58 - 4P, N - [4 - [[2 - [[4 - Cyano - 3 -(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]acet amide 884854-66-4P, 4-[[2-[(Pyrimidin-2-y1)amino]ethy1](2,2,2trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of substituted aniline derivs. as selective androgen receptor

modulators)

884854-00-6 HCAPLUS RN

CN Carbamic acid, [4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2trifluoroethyl)amino]ethoxy]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 884854-06-2 HCAPLUS

Benzoic acid, 4-[2-[[4-cyano-3-(trifluoromethyl)phenyl]](2,2,2-CNtrifluoroethyl)amino]ethoxy]-, methyl ester (CA INDEX NAME)

884854-07-3 HCAPLUS RN

CN Benzoic acid, 4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2trifluoroethyl)amino]ethoxy]- (CA INDEX NAME)

RN 884854-14-2 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(2,2,2-trifluoroacetyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-57-3 HCAPLUS

CN Benzonitrile, 4-[[2-(phenylthio)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CH_2$$
 CF_3 N CH_2 CH_2 CH_2 SPh CH_3

RN 884854-58-4 HCAPLUS

CN Acetamide, N-[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]- (CA INDEX NAME)

RN 884854-66-4 HCAPLUS

CN Benzonitrile, 4-[[2-(2-pyrimidinylamino)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

IT 884853-73-0P, 4-[(Cyclopropylmethyl)[2-[[4-(1,1-dimethylethyl)phenyl]oxy]ethyl]amino]-2-(trifluoromethyl)benzonitrile

```
884853-74-1P, N-[4-[[2-[[4-Cyano-3-(trifluoromethyl)phenyl](cyclop
ropylmethyl)amino]ethyl]oxy]phenyl]acetamide 884853-75-2P,
4-[(Cyclopropylmethyl)[2-[[4-(methyloxy)phenyl]oxy]ethyl]amino]-2-
(trifluoromethyl)benzonitrile 884853-76-3P, 4-
[(Cyclopropylmethyl)[2-[(4-fluorophenyl)oxy]ethyl]amino]-2-
(trifluoromethyl)benzonitrile 884853-77-4P, 4-
[(Cyclopropylmethyl)[2-[[4-(hydroxymethyl)phenyl]oxy]ethyl]amino]-2-
(trifluoromethyl) benzonitrile 884853-78-5P, N-[4-[[3-[[4-Cyano-3-
(trifluoromethyl)phenyl](cyclopropylmethyl)amino]propyl]oxy]phenyl]acetami
de 884853-80-9P, 4-[(Cyclopropylmethyl)[3-[[4-(1,1-
dimethylethyl)phenyl]oxy]propyl]amino]-2-(trifluoromethyl)benzonitrile
884853-81-0P, 4-[(Cyclopropylmethyl)]3-[[4-
(methyloxy)phenyl]oxy]propyl]amino]-2-(trifluoromethyl)benzonitrile
884853-82-1P, 4-[(Cyclopropylmethyl)[3-[(4-
fluorophenyl)oxy]propyl]amino]-2-(trifluoromethyl)benzonitrile
884853-83-2P, 4-[(Cyclopropylmethyl)[3-[[4-
(hydroxymethyl)phenyl]oxy]propyl]amino]-2-(trifluoromethyl)benzonitrile
884853-84-3P, N-[4-[[3-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]propyl]oxy]phenyl]acetamide 884853-85-4P,
4-[[3-[[4-(1,1-Dimethylethyl)phenyl]oxy]propyl](2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884853-86-5P
, 4-[[3-[(4-Fluorophenyl)oxy]propyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884853-87-6P, 4-[[3-[[4-
(Methyloxy)phenyl]oxy]propyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884853-88-7P, 4-[[2-[[4-[[2-(1-1)]]]]]
Piperidinyl)ethyl]oxy]phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884853-89-8P, 4-[[2-[[4-
(Methyloxy)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884853 - 90 - 1P, N-[4-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]phenyl]aceta
mide 884853-91-2P, 4-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]benzenesulfo
namide 884853-92-3P, 4-[[2-[(4-Cyanophenyl))] (2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884853-93-4P
, 4-[[2-[(4-Fluorophenyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884853-94-5P, 4-[[2-[[4-(3-
Oxobutyl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884853-95-6P, 4-[[2-[(1H-Indol-5-100])]
yl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile
884853-96-7P, 4-[[2-[(3-Fluorophenyl)oxy]ethyl](2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884853-97-8P
, 4-[[2-[(4-Acetylphenyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884853-98-9P, 4-[[2-[[4-(2-
Oxopropyl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884853-99-0P, N-[3-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]phenyl]aceta
mide 884854-01-7P, N-[4-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]phenyl]metha
nesulfonamide 884854-03-9P, 1-[4-[[2-[[4-Cyano-3-9]]]]
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]phenyl]urea
884854-04-0P, 4-[[2-[[4-(Methylsulfonyl)phenyl]oxy]ethyl](2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-05-1P
, 4-[(2,2,2-Trifluoroethyl)[2-[[4-(trifluoromethyl)phenyl]oxy]ethyl]amino]-
2-(trifluoromethyl)benzonitrile 884854-08-4P,
4-[[2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]ethyl]oxy]benzamide 884854-09-5P,
1,1-Dimethylethyl [[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl]](2,2,2-
trifluoroethyl)amino]ethyl]oxy]phenyl]methyl]carbamate
884854-12-0P, N-[4-[[2-[[4-Cyano-3-(trifluoromethyl)phenyl]](2,2,2-
trifluoroethyl)amino]ethyl]oxy]phenyl]quanidine trifluoroacetate
```

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884854-15-3P, 4-[(2,2,2-Trifluoroethyl)]2-[[4-[2,2,2-trifluoro-1-
hydroxy-1-(trifluoromethyl)ethyl]phenyl]oxy]ethyl]amino]-2-
(trifluoromethyl)benzonitrile 884854-16-4P, 4-[[2-[[4-(2-0xo-1-1)]]]
pyrrolidinyl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
Thiazol-2-yl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
Oxazol-2-yl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884854-20-0P, 4-[[2-[(2-0xo-
1,2,3,4-tetrahydro-6-quinolinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-21-1P, 4-[[2-(2-
Pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-22-2P,
4-[[2-(3-Pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-23-3P, 4-[[2-(4-1)]
Pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-24-4P, 4-[(2,2,2-
Trifluoroethyl) [2-[[5-(trifluoromethyl)-2-pyridinyl]oxy]ethyl]amino]-2-
(trifluoromethyl)benzonitrile 884854-25-5P, 4-[[2-[(5-Methyl-2-Parthelementhyl)benzonitrile]]
pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-26-6P, 4-[[2-[(6-Chloro-3-
pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-27-7P, 4-[[2-[(6-Methyl-3-1)]]
pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-28-8P, 4-[[2-[(5-Bromo-2-
pyridinyl)oxylethyl](2,2,2-trifluoroethyl)aminol-2-
(trifluoromethyl)benzonitrile 884854-29-9P, 4-[[2-[(6-Fluoro-3-Fluoro-3-Fluoro-3-Fluoro-3-Fluoro-3-Fluoro-3-Fluoro-3-Fluoromethyl)benzonitrile
pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-30-2P, 4-[[2-[(5-Fluoro-2-
pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl) benzonitrile 884854-31-3P, N-[6-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]oxy]-3-
pyridinyl]acetamide 884854-33-5P 884854-36-8P,
4-[[2-(3-Pyridazinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-37-9P, 4-[[2-(4-
Pyrimidinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-60-8P, N-[4-[[2-[[4-Cyano-3-P]]]]
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]-N-
methylacetamide 884854-61-9P, 4-[[2-(Phenylsulfinyl)ethyl](2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-62-0P
N = [4 - [2 - [4 - Cyano - 3 - (trifluoromethyl)phenyl](2, 2, 2 - Cyano - 3 - Cyano - 3
trifluoroethyl)amino]ethyl]sulfinyl]phenyl]acetamide 884854-63-1P
, 4-[[2-(Phenylsulfonyl)ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854 \cdot 64 \cdot 2P, N-[4-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]sulfonyl]phenyl]
acetamide 884854-65-3P, N-[4-[[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]meth
anesulfonamide 884854-67-5P, 4-[[2-[Methyl(pyrimidin-2-
yl)amino]ethyl](2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-68-6P, N-[2-[[4-Cyano-3-
(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]benzamide
884854-69-7P, 4-[[3-(4-Fluorophenyl)propyl](2,2,2-
trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-71-1P
, N-[4-[3-[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-
trifluoroethyl)amino]propyl]phenyl]acetamide 884854-72-2P,
4-[(3-Phenylpropyl)(2,2,2-trifluoroethyl)amino]-2-
(trifluoromethyl)benzonitrile 884854-74-4P 884854-88-0P
884854-89-1P 884854-90-4P 884854-91-5P
884854-92-6P 884854-93-7P 884854-96-0P
884854-97-1P 884854-98-2P 884854-99-3P,
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2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-Nphenylbutanamide 884855-00-9P, 2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(4fluorophenyl)butanamide 884855-01-0P, 4-[[2-(1H-1,2,4-Triazol-1y1)ethy1](2,2,2-trifluoroethy1)amino]-2-(trifluoromethy1)benzonitrile 884855-07-6P 884855-11-2P 884856-05-7P 884856-06-8P 884856-07-9P 884856-08-0P 885050-04-4P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of substituted aniline derivs. as selective androgen receptor modulators) RN 884853-73-0 HCAPLUS Benzonitrile, 4-[(cyclopropylmethyl)[2-[4-(1,1dimethylethyl)phenoxy]ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

CN

RN 884853-74-1 HCAPLUS CN Acetamide, N-[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl) amino]ethoxy]phenyl]- (CA INDEX NAME)

884853-75-2 HCAPLUS RN Benzonitrile, 4-[(cyclopropylmethyl)[2-(4-methoxyphenoxy)ethyl]amino]-2-CN (trifluoromethyl) - (CA INDEX NAME)

RN 884853-76-3 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[2-(4-fluorophenoxy)ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-77-4 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[2-[4-(hydroxymethyl)phenoxy]ethyl]ami no]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-78-5 HCAPLUS

CN Acetamide, N-[4-[3-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl) amino]propoxy]phenyl]- (CA INDEX NAME)

RN 884853-80-9 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[3-[4-(1,1-dimethylethyl)phenoxy]propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-81-0 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[3-(4-methoxyphenoxy)propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-82-1 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[3-(4-fluorophenoxy)propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-83-2 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[3-[4-(hydroxymethyl)phenoxy]propyl]am ino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-84-3 HCAPLUS

CN Acetamide, N-[4-[3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]propoxy]phenyl]- (CA INDEX NAME)

RN 884853-85-4 HCAPLUS

CN Benzonitrile, 4-[[3-[4-(1,1-dimethylethyl)phenoxy]propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-86-5 HCAPLUS

CN Benzonitrile, 4-[[3-(4-fluorophenoxy)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-87-6 HCAPLUS

CN Benzonitrile, 4-[[3-(4-methoxyphenoxy)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-88-7 HCAPLUS

CN Benzonitrile, 4-[[2-[4-[2-(1-piperidinyl)ethoxy]phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-89-8 HCAPLUS

CN Benzonitrile, 4-[[2-(4-methoxyphenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} & \text{CF3} \\ \text{CM}_2 & \text{CH}_2 \\ \text{N} \end{array}$$

RN 884853-90-1 HCAPLUS

CN Acetamide, N-[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)

RN 884853-91-2 HCAPLUS

CN Benzenesulfonamide, 4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]- (CA INDEX NAME)

RN 884853-92-3 HCAPLUS

CN Benzonitrile, 4-[[2-(4-cyanophenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-93-4 HCAPLUS

CN Benzonitrile, 4-[[2-(4-fluorophenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{F}_{3}\text{C-CH}_{2} \\ \text{CH}_{2} \\ \text{CH}_{2} \\ \text{CH}_{2} \\ \end{array}$$

RN 884853-94-5 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(3-oxobutyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$Me = C - CH_2 - CH_2$$

$$F_3 C - CH_2$$

$$CF_3$$

$$CN$$

$$CF_3$$

$$CN$$

RN 884853-95-6 HCAPLUS

CN Benzonitrile, 4-[[2-(1H-indol-5-yloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-96-7 HCAPLUS

CN Benzonitrile, 4-[[2-(3-fluorophenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-97-8 HCAPLUS

CN Benzonitrile, 4-[[2-(4-acetylphenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884853-98-9 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(2-oxopropyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$Me = C + CH_2$$

$$F_3C + CH_2$$

$$CF_3$$

$$CH_2 + CH_2$$

$$CH_2 + CH_2$$

RN 884853-99-0 HCAPLUS

CN Acetamide, N-[3-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)

RN 884854-01-7 HCAPLUS

CN Methanesulfonamide, N-[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl]](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)

$$Me - \bigcup_{N=0}^{\infty} NH$$

$$F_3C - CH_2$$

$$CF_3$$

$$CN$$

RN 884854-03-9 HCAPLUS

CN Urea, N-[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]- (CA INDEX NAME)

RN 884854-04-0 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(methylsulfonyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$Me = \bigcup_{0}^{CF3} F3C - CH2$$

$$CF3$$

$$CN$$

$$CH2 - CH2 - CH2$$

RN 884854-05-1 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[2-[4-(trifluoromethyl)phenoxy]ethyllamino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-08-4 HCAPLUS

CN Benzamide, 4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]- (CA INDEX NAME)

$$H_2N$$
 CF_3 CH_2 CH_2 CH_2 CH_3 CN

RN 884854-09-5 HCAPLUS

CN Carbamic acid, [[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 884854-12-0 HCAPLUS

CN Guanidine, N-[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 884854-11-9 CMF C19 H17 F6 N5 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 884854-15-3 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[2-[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenoxy]ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-16-4 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(2-oxo-1-pyrrolidinyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-17-5 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(2-thiazolyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-19-7 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(2-oxazolyl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$O_{CH_2-CH_2-CH_3}$$

RN 884854-20-0 HCAPLUS

CN Benzonitrile, 4-[[2-[(1,2,3,4-tetrahydro-2-oxo-6-quinolinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-(CA INDEX NAME)

RN 884854-21-1 HCAPLUS

CN Benzonitrile, 4-[[2-(2-pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-22-2 HCAPLUS

CN Benzonitrile, 4-[[2-(3-pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-23-3 HCAPLUS

CN Benzonitrile, 4-[[2-(4-pyridinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-24-4 HCAPLUS

CN Benzonitrile, 4-[(2,2,2-trifluoroethyl)[2-[[5-(trifluoromethyl)-2-pyridinyl]oxy]ethyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-25-5 HCAPLUS

CN Benzonitrile, 4-[[2-[(5-methyl-2-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

Me
$$F_3C-CH_2$$
 CN CN

RN 884854-26-6 HCAPLUS

CN Benzonitrile, 4-[[2-[(6-chloro-3-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-27-7 HCAPLUS

CN Benzonitrile, 4-[[2-[(6-methyl-3-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-28-8 HCAPLUS

CN Benzonitrile, 4-[[2-[(5-bromo-2-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-29-9 HCAPLUS

CN Benzonitrile, 4-[[2-[(6-fluoro-3-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-30-2 HCAPLUS

CN Benzonitrile, 4-[[2-[(5-fluoro-2-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_{3}C-CH_{2}$$

$$CH_{2}$$

$$CH_{2}$$

$$CH_{2}$$

$$CH_{3}$$

RN 884854-31-3 HCAPLUS

CN Acetamide, N-[6-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]-3-pyridinyl]- (CA INDEX NAME)

RN 884854-33-5 HCAPLUS

CN Benzonitrile, 4-[[2-[(1,6-dihydro-6-oxo-3-pyridinyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-36-8 HCAPLUS

CN Benzonitrile, 4-[[2-(3-pyridazinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-37-9 HCAPLUS

CN Benzonitrile, 4-[[2-(4-pyrimidinyloxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-60-8 HCAPLUS

CN Acetamide, N-[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]-N-methyl- (CA INDEX NAME)

RN 884854-61-9 HCAPLUS

CN Benzonitrile, 4-[[2-(phenylsulfinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-62-0 HCAPLUS

CN Acetamide, N-[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]sulfinyl]phenyl]- (CA INDEX NAME)

RN 884854-63-1 HCAPLUS

CN Benzonitrile, 4-[[2-(phenylsulfonyl)ethyl](2,2,2-trifluoroethyl)amino]-2-

(trifluoromethyl) - (CA INDEX NAME)

RN 884854-64-2 HCAPLUS

CN Acetamide, N-[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]sulfonyl]phenyl]- (CA INDEX NAME)

RN 884854-65-3 HCAPLUS

CN Methanesulfonamide, N-[4-[[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]thio]phenyl]- (CA INDEX NAME)

$$Me = \bigcup_{S=S}^{O} NH$$

$$F_3C - CH_2$$

$$S - CH_2 - CH_2 - N$$

$$CN$$

RN 884854-67-5 HCAPLUS

CN Benzonitrile, 4-[[2-(methyl-2-pyrimidinylamino)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-68-6 HCAPLUS

CN Benzamide, N-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)

RN 884854-69-7 HCAPLUS

CN Benzonitrile, 4-[[3-(4-fluorophenyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-71-1 HCAPLUS

CN Acetamide, N-[4-[3-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]propyl]phenyl]- (CA INDEX NAME)

RN 884854-72-2 HCAPLUS

CN Benzonitrile, 4-[(3-phenylpropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CF_3$$
 $N = (CH_2)_3 = Ph$
 $F_3C = CH_2$

RN 884854-74-4 HCAPLUS

CN Benzonitrile, 4-[[3-(3-pyridinyl)propyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 884854-73-3 CMF C18 H15 F6 N3

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 884854-88-0 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-(4-fluorophenyl)- (CA INDEX NAME)

RN 884854-89-1 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-[(4-fluorophenyl)methyl]- (CA INDEX NAME)

RN 884854-90-4 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-[(1S)-1-phenylethyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 884854-91-5 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-(2-phenylethyl)- (CA INDEX NAME)

RN 884854-92-6 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]- N-[2-(4-fluorophenyl)ethyl]- (CA INDEX NAME)

RN 884854-93-7 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]-N-(4-fluorophenyl)- (CA INDEX NAME)

RN 884854-96-0 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-phenyl- (CA INDEX NAME)

RN 884854-97-1 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(4-fluorophenyl)- (CA INDEX NAME)

RN 884854-98-2 HCAPLUS

CN Acetamide, N-[4-(acetylamino)phenyl]-2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 884854-99-3 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-phenyl- (CA INDEX NAME)

RN 884855-00-9 HCAPLUS

CN Butanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]-N-(4-fluorophenyl)- (CA INDEX NAME)

RN 884855-01-0 HCAPLUS

CN Benzonitrile, 4-[[2-(1H-1,2,4-triazol-1-yl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884855-07-6 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[2-(4-morpholinyl)ethyl]amino]-2-(trifluoromethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 884855-06-5 CMF C18 H22 F3 N3 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 884855-11-2 HCAPLUS

CN Benzonitrile, 4-[[2-(1-pyrrolidinyl)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 884855-10-1 CMF C16 H17 F6 N3

CM 2

CRN 76-05-1

CMF C2 H F3 O2

RN 884856-05-7 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-phenyl- (CA INDEX NAME)

RN 884856-06-8 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]-N-(phenylmethyl)- (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_3

RN 884856-07-9 HCAPLUS

CN Propanamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amin o]-N-phenyl- (CA INDEX NAME)

RN 884856-08-0 HCAPLUS

CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-

trifluoroethyl)amino]-N-(2-phenylethyl)- (CA INDEX NAME)

RN 885050-04-4 HCAPLUS
CN Acetamide, 2-[[4-cyano-3-(trifluoromethyl)phenyl](cyclopropylmethyl)amino]N-[(1R)-1-phenylethyl]- (CA INDEX NAME)

Absolute stereochemistry.

821777-25-7P, 4-[(Cyclopropylmethyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)benzonitrile 821777-26-8P, 4-[(Cyclopropylmethyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)benzonitrile 821777-52-09, 4-[(3-Hydroxypropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 821777-58-6P, 4-[(2-Hydroxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 821777-73-5P 821777-85-9P, 2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl methanesulfonate 821777-86-0P, 4-[(2-Aminoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 864283-36-3P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)qlycine 864283-47-6P , N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)qlycine 864283-49-8P, Methyl N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)glycinate 864283-71-6P, 2-[[4-Cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]butanoic acid 864284-25-3P, N-[4-Cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)alanine 884854-02-8P, 4-[[2-[(4-Aminophenyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-10-8P, 4-[[2-[(4-Formylphenyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-13-1P 884854-18-6P , 4-[[2-[[4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2yl)phenyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-35-7P, 4-[[2-[[6-[[4-(Methyloxy)phenyl]methyl]oxy]-3-pyridinyl]oxy]ethyl](2,2,2trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile 884854-59-5P , 4-[[2-[(4-Aminophenyl)thio]ethyl](2,2,2-trifluoroethyl)amino]-2-

(trifluoromethyl)benzonitrile 884854-70-0P, 4-[(2-Propen-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)benzonitrile RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted aniline derivs. as selective androgen receptor modulators)

RN 821777-25-7 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-26-8 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-52-0 HCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-58-6 HCAPLUS

CN Benzonitrile, 4-[(2-hydroxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-73-5 HCAPLUS

CN Benzonitrile, 4-[(2-azidoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-85-9 HCAPLUS

CN Benzonitrile, 4-[[2-[(methylsulfonyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-86-0 HCAPLUS

CN Benzonitrile, 4-[(2-aminoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 864283-36-3 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 864283-47-6 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-(CA INDEX NAME)

RN 864283-49-8 HCAPLUS

CN Glycine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(2,2,2-trifluoroethyl)-, methyl ester (CA INDEX NAME)

$$CN$$
 CF_3
 $N-CH_2-C-OMe$
 F_3C-CH_2
 CF_3

RN 864283-71-6 HCAPLUS

CN Butanoic acid, 2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

RN 864284-25-3 HCAPLUS

CN Alanine, N-[4-cyano-3-(trifluoromethyl)phenyl]-N-(cyclopropylmethyl)- (CA INDEX NAME)

RN 884854-02-8 HCAPLUS

CN Benzonitrile, 4-[[2-(4-aminophenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-10-8 HCAPLUS

CN Benzonitrile, 4-[[2-(4-formylphenoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-13-1 HCAPLUS

CN Carbamic acid, [[4-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethoxy]phenyl]carbonimidoyl]bis-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 884854-18-6 HCAPLUS

CN Benzonitrile, 4-[[2-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenoxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 884854-35-7 HCAPLUS

CN Benzonitrile, 4-[[2-[[6-[(4-methoxyphenyl)methoxy]-3-pyridinyl]oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CF}_3 \\ \text{NC} \\ \begin{array}{c} \text{CH}_2 - \text{CF}_3 \\ \text{N-CH}_2 - \text{CH}_2 - \text{O} \\ \end{array} \\ \begin{array}{c} \text{N} \\ \text{O-CH}_2 \end{array} \\ \end{array} \\ \begin{array}{c} \text{OMe} \\ \end{array}$$

RN 884854-59-5 HCAPLUS

CN Benzonitrile, 4-[[2-[(4-aminophenyl)thio]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$F_3C-CH_2$$
 CF_3
 CN
 $S-CH_2-CH_2-N$

RN 884854-70-0 HCAPLUS

CN Benzonitrile, 4-[2-propen-1-yl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CF_3$$
 N
 CF_3
 N
 CH_2
 CH_2
 CH_2

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:14359 HCAPLUS Full-text

DOCUMENT NUMBER: 142:113710

TITLE: Preparation of substituted anilines as androgen

receptor modulators

INVENTOR(S):
Blanc, Jean-Baptiste E.; Cadilla, Rodolfo;

Cowan, David John; Kaldor, Istvan; Larkin, Andrew L.; Stewart, Eugene Lee

; Turnbull, Philip Stewart; Trump, Ryan Paul

PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.					D	DATE		APPLICATION NO.						DATE			
		2005000795 2005000795								WO 2004-US18252								
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		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	
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OTHER SOURCE(S): MARPAT 142:113710

ED Entered STN: 07 Jan 2005

GΙ

This invention relates to non-steroidal compds. I [R1, R2, R4, R5 = H, CN, NO2, halo, etc. (at least one of R1, R2, R4, R5 is not H); R3 = CN, NO2, halo, etc.; R6, R7 = H, (Ra)xR9 (Ra = alkylene; x = 0-1; R9 = alkyl, haloalkyl, hydroxyalkyl, etc.)] that are or are believed to be modulators of androgen, glucocorticoid, mineralocorticoid, and progesterone receptors, and also to the methods for the making and use of such compds. Thus, reacting 4-fluoro-2-trifluoromethylbenzonitrile with N-(cyclopropylmethyl)-N-propylamine afforded 81% I [R1, R2, R5 = H; R3 = CN; R4 = CF3; R6 = CH2(cyclopropyl); R7 = Pr]. The compds. I are claimed to be useful in the treatment or prophylaxis of conditions or disorders that respond to selective androgen receptor modulation (no data given). The pharmaceutical composition comprising the compound I is disclosed.

IT 821777-58-6P 821777-66-6P 821777-68-8P 821777-73-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted anilines as androgen receptor modulators)

RN 821777-58-6 HCAPLUS

CN Benzonitrile, 4-[(2-hydroxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CH_2$$
 CF_3 CH_2 CH_2 CH_2 CH_3

RN 821777-66-6 HCAPLUS

CN Benzonitrile, 4-[(2-methyl-2-propen-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-68-8 HCAPLUS

CN Benzonitrile, 4-[(3-methyl-2-buten-1-yl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-73-5 HCAPLUS

CN Benzonitrile, 4-[(2-azidoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

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821776-43-6P 821776-44-7P 821776-58-3P
     821777-25-7P 821777-26-8P 821777-33-7P
     821777-52-0P 821777-55-3P 821777-56-4P
     821777-59-7P 821777-60-0P 821777-61-1P
     821777-62-2P 821777-63-3P 821777-64-4P
     821777-65-5P 821777-67-7P 821777-69-9P
     821777-70-2P 821777-71-3P 821777-72-4P
     821777-74-6P 821777-75-7P 821777-76-8P
     821777-77-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of substituted anilines as androgen receptor modulators)
RN
     821776-43-6 HCAPLUS
     Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-(trifluoromethyl)- (CA
CN
```

INDEX NAME)

RN 821776-44-7 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)propylamino]-2-nitro- (CA INDEX NAME)

RN 821776-58-3 HCAPLUS

CN Benzonitrile, 2-chloro-4-[(cyclopropylmethyl)propylamino]- (CA INDEX NAME)

RN 821777-25-7 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(3-hydroxypropyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CH_2-N$$
 CF_3

RN 821777-26-8 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(2-hydroxyethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-33-7 HCAPLUS

CN Benzonitrile, 4-[(1-cyclopropylethyl)-2-propen-1-ylamino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-52-0 HCAPLUS

CN Benzonitrile, 4-[(3-hydroxypropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-55-3 HCAPLUS

CN Benzonitrile, 4-[bis(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-56-4 HCAPLUS

CN Benzonitrile, 4-[(2,2-difluoroethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-59-7 HCAPLUS

CN Benzonitrile, 4-[(2-methoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-60-0 HCAPLUS

CN Benzonitrile, 4-[(2-ethoxyethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CF_3$$
 $N=CH_2=CH_2=OEt$
 $F_3C=CH_2$

RN 821777-61-1 HCAPLUS

CN Benzonitrile, 4-[[2-(2,2,2-trifluoroethoxy)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-62-2 HCAPLUS

CN Benzonitrile, 4-[methyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-63-3 HCAPLUS

CN Benzonitrile, 4-[ethyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-(CA INDEX NAME)

RN 821777-64-4 HCAPLUS

CN Benzonitrile, 4-[propyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)-(CA INDEX NAME)

RN 821777-65-5 HCAPLUS

CN Benzonitrile, 4-[butyl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-67-7 HCAPLUS

CN Benzonitrile, 4-[(2-methylpropyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-69-9 HCAPLUS

CN Benzonitrile, 4-[(3-methylbutyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-70-2 HCAPLUS

CN Benzonitrile, 4-[2-propyn-1-yl(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-71-3 HCAPLUS

CN Benzonitrile, 4-[(2-fluoroethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-72-4 HCAPLUS

CN Benzonitrile, 4-[[2-(methylthio)ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

$$CF_3$$
 N
 CF_3
 N
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

RN 821777-74-6 HCAPLUS

CN Acetamide, N-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)

RN 821777-75-7 HCAPLUS

CN Carbamic acid, [2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 821777-76-8 HCAPLUS

CN Carbamic acid, [2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 821777-77-9 HCAPLUS

CN Methanesulfonamide, N-[2-[[4-cyano-3-(trifluoromethyl)phenyl](2,2,2-trifluoroethyl)amino]ethyl]- (CA INDEX NAME)

$$CF_3$$
 N
 CF_3
 N
 CH_2
 CH_2
 CH_2
 CH_3
 CH_4
 CH_5
 CH_5
 CH_5
 CH_6
 CH_6
 CH_7
 CH_7

IT 821777-79-1P 821777-85-9P 821777-86-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted anilines as androgen receptor modulators)

RN 821777-79-1 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]propyl]amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-85-9 HCAPLUS

CN Benzonitrile, 4-[[2-[(methylsulfonyl)oxy]ethyl](2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN 821777-86-0 HCAPLUS

CN Benzonitrile, 4-[(2-aminoethyl)(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

Author Search

=> FILE HCAPLUS

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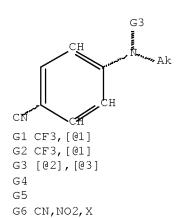
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'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> D STAT QUE L4 L1 STR

G2³ Cy ¹

 $Ak^2 G1$



Structure attributes must be viewed using STN Express query preparation. L3 774 SEA FILE=REGISTRY SSS FUL L1

L437 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> D STAT QUE L7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. 189) SEA FILE=REGISTRY SSS FUL L5

L7 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L6

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 $G2^3$ Cy^1

 $Ak_{\underline{2}}G1$

G1 CF3, [@1]

G2 CF3, [@1] G3 [@2],[@3]

G4

G5

G6 CN, NO2, X

Structure attributes must be viewed using STN Express query preparation.

774 SEA FILE=REGISTRY SSS FUL L1 L3

L10 STR $G2^3$ Cy 1

 $Ak^2 G1$

Structure attributes must be viewed using STN Express query preparation.

L12 395 SEA FILE=REGISTRY SUB=L3 SSS FUL L10 L13 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L12

=> S L13,L7,L4 NOT L34

L42 31 (L13 OR L7 OR L4) NOT L34

=> FILE WPIX

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MOST RECENT UPDATE: 200860 <200860/DW>
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20071130/UPIC, 20080401/UPIC and 20080701/UPIC.
ECLA reclassifications to June and US national classifications to
the end of April 2008 have also been loaded. Update dates
20080401 and 20080701/UPEC and /UPNC have been assigned to these. <<</pre>

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'BI, ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE
=> D STAT QUE L37
1.8
               STR
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.
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L36
L37
             2 SEA FILE=WPIX ABB=ON PLU=ON L36/DCR
=> S L37 NOT L38
            0 L37 NOT L38
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L43 HAS NO ANSWERS
L40 HAS NO ANSWERS
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FILE COVERS 1907 - 26 Sep 2008 VOL 149 ISS 14 FILE LAST UPDATED: 25 Sep 2008 (20080925/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

PROCESSING COMPLETED FOR L42 PROCESSING COMPLETED FOR L43 PROCESSING COMPLETED FOR L40

L44 31 DUP REM L42 L43 L40 (0 DUPLICATES REMOVED)

ANSWERS '1-31' FROM FILE HCAPLUS

=> D IBIB ED ABS HITSTR L44 1-31

L44 ANSWER 1 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:962643 HCAPLUS Full-text

TITLE: Potent, Plasmodium-Selective Farnesyltransferase Inhibitors That Arrest the Growth of Malaria

Parasites: Structure-Activity Relationships of Ethylenediamine-Analogue Scaffolds and Homology Model

Validation

AUTHOR(S): Fletcher, Steven; Cummings, Christopher G.; Rivas,

Kasey; Katt, William P.; Horney, Carrie; Buckner, Frederick S.; Chakrabarti, Debopam; Sebti, Said M.; Gelb, Michael H.; Van Voorhis, Wesley C.; Hamilton,

Andrew D.

CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,

CT, 06511, USA

SOURCE: Journal of Medicinal Chemistry (2008), 51(17),

5176-5197

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 11 Aug 2008

AB New chemotherapeutics are urgently needed to combat malaria. We previously reported on a novel series of antimalarial, ethylenediamine-based inhibitors of protein farnesyltransferase (PFT). In the current study, we designed and synthesized a series of second generation inhibitors, wherein the core ethylenediamine scaffold was varied in order to examine both the homol. model of Plasmodium falciparum PFT (PfPFT) and our predicted inhibitor binding mode. We identified several PfPFT inhibitors (PfPFTIs) that are selective for PfPFT vs. the mammalian isoform of the enzyme (up to 136-fold selectivity), that inhibit the malarial enzyme with IC50 values down to 1 nM, and that block the growth of P. falciparum in infected whole cells (erythrocytes) with ED50 values down to 55 nM. The structure-activity data for these second generation, ethylenediamine-inspired PFT inhibitors were rationalized by consideration of the X-ray crystal structure of mammalian PFT and the homol. model of the malarial enzyme.

IT 910910-63-3P 1052099-95-2P 1052099-96-3P 1052099-97-4P 1052099-98-5P 1052099-99-6P 1052100-00-1P 1052100-01-2P 1052100-02-3P 1052100-03-4P 1052100-04-5P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(plasmodium-selective farnesyltransferase inhibitors that arrest malaria parasites growth: SAR of ethylenediamine analog scaffolds and homol. model validation)

RN 910910-63-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[1-(2-pyrimidinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} & \text{NMe} \\ \text{NMe} & \text{OSSO} & \text{NMe} \\ \text{NMe} & \text{CH}_2 - \text{NH}_2 - \text{CH}_2 - \text{NH}_2 - \text{CH}_2 \\ \text{NMe} & \text{NMe} & \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} \\ \text{NMe} & \text{NMe} \\ \text{NMe} \\ \text{NMe} \\$$

RN 1052099-95-2 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$CH_2$$
—Ph

 CH_2 —N— $(CH_2)_3$ —N— CH_2 —Ph

 Me

RN 1052099-96-3 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

Me O
$$CH_2$$
 Me N CH_2 CH_2

RN 1052099-97-4 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

RN 1052099-98-5 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

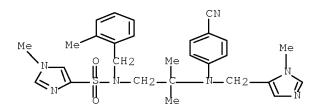
RN 1052099-99-6 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - (\text{CH}_2)_3 - \text{N} - \text{CH}_2 \end{array}$$

RN 1052100-00-1 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} CN \\ \hline \\ N \\ \hline \\ N \\ \hline \\ CH_2-N \\ \hline \\ Me \\ \hline \\ CH_2-Ph \\ \hline \\ CH_2-Ph \\ \hline \\ O \\ \hline \\ N \\ \hline \\ Me \\ \hline \end{array}$$

RN 1052100-01-2 HCAPLUS CN INDEX NAME NOT YET ASSIGNED



RN 1052100-02-3 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & & & \\ & & & \\ N & & \\ N & & \\ N & & \\ CH_2 - N & & \\ Me & & \\ Me & & \\ \end{array} \begin{array}{c} & \\ CH_2 & \\ CH_2 & \\ N & \\ N & \\ \end{array} \begin{array}{c} \\ Me \\ N & \\ N$$

RN 1052100-03-4 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-04-5 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

IT 865788-27-8 865788-35-8 910910-62-2 1052099-94-1

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(plasmodium-selective farnesyltransferase inhibitors that arrest malaria parasites growth: SAR of ethylenediamine analog scaffolds and homol. model validation)

RN 865788-27-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2\text{-Ph} \\ \text{O} \\ \text{N} \\ \text{Me} \end{array}$$

RN 865788-35-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(2-methylphenyl)methyl]- (CA INDEX NAME)

RN 910910-62-2 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 1052099-94-1 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \stackrel{\text{Me}}{\longleftarrow} & \stackrel{\text{Ch}}{\longleftarrow} & \stackrel{\text{Ch}}{\longrightarrow} & \stackrel{\text{Ch}}{\longrightarrow} & \stackrel{\text{Me}}{\longrightarrow} & \stackrel{\text{Me}}{\longrightarrow} & \stackrel{\text{Me}}{\longrightarrow} & \stackrel{\text{Ch}}{\longrightarrow} & \stackrel{\text{Ch}}{$$

IT 1052100-30-7P 1052100-31-8P 1052100-40-9P 1052100-41-0P 1052100-44-3P 1052100-45-4P 1052100-46-5P 1052100-47-6P 1052100-48-7P

1052100-49-8P 1052100-50-1P 1052100-51-2P 1052100-52-3P 1052100-54-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(plasmodium-selective farnesyltransferase inhibitors that arrest malaria parasites growth: SAR of ethylenediamine analog scaffolds and homol. model validation)

RN 1052100-30-7 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2 - \text{N} \\
\text{(CH}_2)_3
\end{array}$$

RN 1052100-31-8 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

RN 1052100-40-9 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-41-0 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-44-3 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} O \\ C - CH_2 - O - CH_2 - Ph \end{array}$$

RN 1052100-45-4 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-46-5 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-47-6 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

Me N CH2 CH2
$$\stackrel{\text{CN}}{\longrightarrow}$$
 $\stackrel{\text{Me}}{\longrightarrow}$ $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{\text{CH}_2}{\longrightarrow}$ $\stackrel{\text{CH}_2}{\longrightarrow}$ $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{\text{CH}_2}{\longrightarrow}$ $\stackrel{\text{N}}{\longrightarrow}$ $\stackrel{\text{N$

RN 1052100-48-7 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-49-8 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} CN \\ \downarrow \\ N \\ \downarrow \\ N \\ Me \end{array} \quad \begin{array}{c} CH_2 \\ \downarrow \\ N \\ CH_2 \\ \end{array} \quad \begin{array}{c} CH_2 \\ \downarrow \\ CH_2 \\ \end{array} \quad \begin{array}{c} CH_2 \\ \downarrow \\ CH_2 \\ \end{array} \quad \begin{array}{c} CH_2 \\ \downarrow \\ \end{array} \quad \begin{array}{c} C$$

RN 1052100-50-1 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{CH}_2-\text{NH}_2}{\bigvee}} & \overset{\text{CN}}{\underset{\text{CH}_2-\text{CH}_2-\text{NH}_2}{\bigvee}} & \overset{\text{O}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{N}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{CH}_2-\text{NH}_2}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}{\bigvee}} & \overset{\text{CN}}{\underset{\text{Me}}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}{\underset{\text{Me}}}{\underset{\text{Me}}{\underset{\text{Me}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}}{\underset{\text{Me}}}}{$$

RN 1052100-51-2 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 1052100-52-3 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 1052100-54-5 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:761566 HCAPLUS Full-text

DOCUMENT NUMBER: 147:166201

TITLE: Preparation of 3,5-Substituted Piperidine Compounds as

Renin Inhibitors

INVENTOR(S): Ehara, Takeru; Grosche, Philipp; Irie, Osamu; Iwaki,

Yuki; Kanazawa, Takanori; Kawakami, Shimpei; Konishi,

Kazuhide; Mogi, Muneto; Suzuki, Masaki; Yokokawa,

Fumiaki

PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH

SOURCE: PCT Int. Appl., 692pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	CENT	NO.			KIND DATE			-	APPL	ICAT	ION 1		DATE						
WO	2007	A1	_	2007	0712	,	WO 2	 006-	EP12		20061228								
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,		
		KΡ,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,		
		MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NΙ,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,		
		RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ΤJ,	TM,	TN,	TR,	TT,		
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW								
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,		
		IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,		
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	ΤG,	BW,	GH,		
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,	ΑZ,	BY,		
		KG,	KΖ,	MD,	RU,	ТJ,	TM												
AU	AU 2006332124						2007	0712		AU 2	006-	3321	20061228						
EP	EP 1968940					A1 20080917				EP 2	006-	82989	20061228						
	R:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,		
		IS,	ΙΤ,	LI,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BA,	HR	
ORITY APPLN. INFO.:									EP 2005-28771						A 20051230				
	GB 2006-4223							A 20060302											
						GB 2006-11390						0	A 20060608						
									,	WO 2	006-	EP12.	581	,	W 2	0061	228		
IDD O	NANDI		1 17.	1000	Λ1														

OTHER SOURCE(S): MARPAT 147:166201

ED Entered STN: 13 Jul 2007

GI

AΒ Title compds. I [R1 = H, (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = (un) substituted alkyl, alkenyl, alkynyl, aryl, etc.; R3 = H, (un) substituted aryl or alkyl; R4 = (un)substituted alkyl, alkenyl, aryl, heterocyclyl, etc.; or R3 and R4 may together form (un) substituted nitrogen heterocycle; R6 = H, halo, alkyl or alkoxy; R7 and R8 independently = H or halo; T = methylene or carbonyl], and their pharmaceutically acceptable salts, are disclosed as renin inhibitors and as such are useful for the treatment of a disease (= disorder) that depends on activity of renin. Thus, e.g., II was prepared in a multistep synthesis from indole-3-carboxaldehyde via N-alkylation with toluene-4sulfonic acid 3-methoxypropyl ester followed by reductive amination with cyclopropyl amine, reaction with 2,4-dioxo-3-oxa-7-aza- bicyclo[3.3.1]nonane-7-carboxylic acid tert Bu ester, amidation with isobutylamine and deprotection. I in assays for inhibition of recombinant human renin will preferably possess IC50 values in the range from 1 nM to 20 μM (no data). Further disclosed are methods for preparation of a pharmaceutical formulation for the treatment of a disease that depends on activity of renin.

IT 944137-09-1P 944137-10-4P 944137-29-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted piperidine compds. as renin inhibitors)

RN 944137-09-1 HCAPLUS

3,5-Piperidinedicarboxamide, N3-[4-cyano-3-(3-methoxypropoxy)phenyl]-N3cyclopropyl-N5-[3-methyl-1-(2-methylpropyl)butyl]-, (3R,5S)-rel- (CA
INDEX NAME)

Relative stereochemistry.

RN 944137-10-4 HCAPLUS

CN 3,5-Piperidinedicarboxamide, N3-[4-cyano-3-(3-methoxypropoxy)phenyl]-N3-cyclopropyl-N5-(2-methoxy-6-methylphenyl)-, (3R,5S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 944137-29-5 HCAPLUS

CN 3,5-Piperidinedicarboxamide, N3-[4-cyano-3-(3-methoxypropoxy)phenyl]-N3-cyclopropyl-N5-[1-(4-pyridinyl)cyclopentyl]-, (3R,5S)- (CA INDEX NAME)

Absolute stereochemistry.

IT 944142-31-8P 944142-32-9P 944142-34-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of substituted piperidine compds. as renin inhibitors)

RN 944142-31-8 HCAPLUS

CN 1-Piperidinecarboxylic acid, 3-[[[4-cyano-3-(3-methoxypropoxy)phenyl]cyclopropylamino]carbonyl]-5-[[[1-(4-pyridinyl)cyclopentyl]amino]carbonyl]-, 1,1-dimethylethyl ester, (3R,5S)-(CA INDEX NAME)

Absolute stereochemistry.

RN 944142-32-9 HCAPLUS

CN 1,3-Piperidinedicarboxylic acid, 5-[[[4-cyano-3-(3-methoxypropoxy)phenyl]cyclopropylamino]carbonyl]-, 1-(1,1-dimethylethyl) ester, (3S,5R)- (CA INDEX NAME)

Absolute stereochemistry.

RN 944142-34-1 HCAPLUS

CN 1,3-Piperidinedicarboxylic acid, 5-[[[4-cyano-3-(3-methoxypropoxy)phenyl]cyclopropylamino]carbonyl]-, 1-(1,1-dimethylethyl) 3-methyl ester, (3S,5R)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 3 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:538978 HCAPLUS Full-text

DOCUMENT NUMBER: 146:521801

TITLE: Preparation of 1-N-phenyl-amino-1H-imidazole derivatives as aromatase, steroid sulfatase, and

carbonic anhydrase inhibitors and pharmaceutical

compositions containing them

INVENTOR(S): Lafay, Jean; Rondot, Benoit; Bonnet, Paule; Clerc,

Thierry; Shields, Jaqueline; Duc, Igor; Duranti, Eric; Puccio, Francois; Blot, Christian; Maillos, Philippe

PATENT ASSIGNEE(S): Fr.

SOURCE: U.S. Pat. Appl. Publ., 32pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

	PATENT NO.						KIND DATE			APPLICATION NO.							DATE			
	US	2007	A1	_	2007	0517		 US 2	2006-	20060817										
	EP 1544195			A1 20050			0622		EP 2	003-		20031215								
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,		
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	ΑL,	TR,	BG,	CZ,	EE,	HU,	SK			
	WO 2005058842				A1		2005	0630		WO 2	004-		20041215							
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,		
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,		
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
			ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,		
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,		
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,		
			MR,	ΝE,	SN,	TD,	ΤG													
PRIO	PRIORITY APPLN. INFO.:										EP 2	003-	2931	52		A 2	0031	215		
											EP 2	004-	2926	81		A 2	0041	112		
											WO 2	004-	EP14	847		W 2	0041	215		
OTHER	OTHER SOURCE(S):						MARPAT 146:521801													

ED Entered STN: 18 May 2007

GΙ

AΒ The invention relates to the compds. of formula I: in which R1 and R2 are H, (C1-C6)alkyl, (C3-C8)cycloalkyl, or together form a (un)saturated 5-7-membered carbocyclic ring; Q is (CH2)m-X-(CH2)n-A; A is a direct link, O, S, SO, SO2, NR5; X is a direct link, CF2, O, S, SO, SO2, C(O), NR5 or CR6R7; Z is (un) substituted Ph or heterocycle; m and n are 0-4; R3 is H, OH, (C1-C6) alkyl, etc.; R4 is H, OH, CN, halo, (C1-C6)alkoxy, etc.; R3 and R4 together with the Ph ring bearing them can also form a benzofuran or a N-methylbenzotriazole; R6 and R7 are H, halo, (C1-C6)alkyl or (C3-C8) cycloalkyl; R5, is H, OH, (C1-C6)alkyl, or (C3-C8)cycloalkyl;. I are inhibitors of the enzymes aromatase and/ or steroid sulfatase and/or carbonic anhydrase and can be used alone or in combination with other active ingredients for the treatment or the prevention of any hormone or non hormone-dependent cancer, in humans as well as in wild or domestic animals. Because of their inhibition activity of aromatase and/or steroid sulfatase, the compds. of the invention are suitable for the management of estrogen-regulated reproductive functions, in humans as well as in wild or domestic animals. The invention also relates to the pharmaceutical compns. containing these compds. Example compound, 4-[N-(4hydroxyphenylmethyl) - N-(1H-imidazol-1-yl)amino]benzonitrile (II) , was

prepared by reacting 4-hydroxybenzyl bromide and 4-[N-(1H-imidazol-1-yl)] amino]benzonitrile. II inhibited human aromatase with IC50 = 0.17 nM. 936575-69-8P

RL: BYP (Byproduct); PREP (Preparation) (drug candidate; preparation of 1-N-Ph-amino-1H-imidazole derivs. as aromatase, steroid sulfatase, and carbonic anhydrase inhibitors and pharmaceutical compns. containing them)

RN 936575-69-8 HCAPLUS

CN Sulfamic acid, N-(aminosulfonyl)-, compd. with 4-[[(3-bromophenyl)methyl]-1H-imidazol-1-ylamino|benzonitrile (1:1) (CA INDEX NAME)

CM 1

ΙT

CRN 936575-68-7 CMF C17 H13 Br N4

CM 2

CRN 13776-65-3 CMF H4 N2 O5 S2

IT 854602-62-3P, 4-[N-(4-Hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-63-4P, 4-[N-(3-Chloro-4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-64-5P, 4-[N-(3-Bromo-4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-65-6P, 4-[N-[(4-Hydroxy-3-methoxyphenyl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-67-8P, 4-[N-(3-Formyl-4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-76-9P, 4-[N-[(2,2-Dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile 936575-31-4P, 4-[N-[2-(4-Benzyloxyphenoxy)ethyl]-N-(1H-imidazol-1-yl)amino]benzonitrile 936575-38-1P, N-(1H-imidazol-1-yl)amino]benzonitrile 936575-38-1P, N-(1H-Imidazol-1-yl)-N-(4-cyanophenyl)-2-(4-hydroxyphenyl)acetamide 936575-39-2P, N-(4-Cyanophenyl)-3-(4-

hydroxyphenyl)-N-(1H-imidazol-1-yl)propanamide 936575-41-6P, 5-Nitro-N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)benzothiophene-2-carboxamide 936575-42-7P, N-(4-Cyanophenyl)-N-(1H-imidazol-1-yl)-2-(6methoxybenzo[b]thien-3-yl)acetamide 936575-43-8P, 4-[N-(1H-Imidazol-1-yl)-N-[(6-methoxybenzo[b]thien-3yl)methyl]amino]benzonitrile 936575-45-0P, 4-[N-[(6-Benzyloxybenzo[b]thien-2-yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile 936575-46-1P, 4-[N-[(6-Hydroxybenzo[b]thien-3-yl)methyl]-N-(1H-1)imidazol-1-yl)amino]benzonitrile 936575-49-4P, 4-[N-[2-(4-Hydroxyphenoxy)ethyl]-N-(1H-imidazol-1-yl)amino]benzonitrile936575-52-9P, 4-[N-[(6-Hydroxybenzo[b]thien-2-y1)methy1]-N-(1Himidazol-1-yl)amino]benzonitrile 936575-54-1P, 5-Amino-N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)benzothiophene-2-carboxamide 936575-73-4P, 4-[N-[(2,2-Dioxido-3-tosyl-3H-1,2,3-benzoxathiazol-5-five]yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (drug candidate; preparation of 1-N-Ph-amino-1H-imidazole derivs. as aromatase, steroid sulfatase, and carbonic anhydrase inhibitors and pharmaceutical compns. containing them) 854602-62-3 HCAPLUS Benzonitrile, 4-[[(4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA

INDEX NAME)

RN CN

RN 854602-63-4 HCAPLUS
CN Benzonitrile, 4-[[(3-chloro-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino](CA INDEX NAME)

RN 854602-64-5 HCAPLUS

CN Benzonitrile, 4-[[(3-bromo-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-65-6 HCAPLUS

CN Benzonitrile, 4-[[(4-hydroxy-3-methoxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-67-8 HCAPLUS

CN Benzonitrile, 4-[[(3-formyl-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

CN Benzonitrile, 4-[[(2,2-dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-31-4 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[2-[4-(phenylmethoxy)phenoxy]ethyl]amino]- (CA INDEX NAME)

RN 936575-34-7 HCAPLUS

CN Benzonitrile, 4-[[(4-hydroxy-3-nitrophenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN

CN Benzeneacetamide, N-(4-cyanophenyl)-4-hydroxy-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-39-2 HCAPLUS

CN Benzenepropanamide, N-(4-cyanophenyl)-4-hydroxy-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-41-6 HCAPLUS

CN Benzo[b]thiophene-2-carboxamide, N-(4-cyanophenyl)-N-1H-imidazol-1-yl-5-nitro- (CA INDEX NAME)

CN Benzo[b]thiophene-3-acetamide, N-(4-cyanophenyl)-N-1H-imidazol-1-yl-6-methoxy- (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \\ \end{array} \begin{array}{c} \text{S} \\ \\ \end{array} \begin{array}{c} \text{CH}_2 \\ \end{array} \begin{array}{c} \text{CN} \\ \\ \end{array} \begin{array}{c} \text{N} \\ \\ \end{array} \begin{array}{c} \text{N} \\ \end{array} \begin{array}{c} \text{N} \\ \end{array}$$

RN 936575-43-8 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[(6-methoxybenzo[b]thien-3-yl)methyl]amino]- (CA INDEX NAME)

RN 936575-45-0 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[[6-(phenylmethoxy)benzo[b]thien-2-yl]methyl]amino]- (CA INDEX NAME)

RN 936575-46-1 HCAPLUS

CN Benzonitrile, 4-[[(6-hydroxybenzo[b]thien-3-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

HO
$$CH_2$$
 N N

RN 936575-49-4 HCAPLUS

CN Benzonitrile, 4-[[2-(4-hydroxyphenoxy)ethyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-52-9 HCAPLUS

CN Benzonitrile, 4-[[(6-hydroxybenzo[b]thien-2-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-54-1 HCAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-amino-N-(4-cyanophenyl)-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-73-4 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[[3-[(4-methylphenyl)sulfonyl]-2,2-[]]

dioxido-3H-1,2,3-benzoxathiazol-5-yl]methyl]amino]- (CA INDEX NAME)

$$N = N - CH_2$$

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854602-71-4P, Sulfamic acid 4-[[N-(4-cyanophenyl)-N-(1H-imidazol-1-1)]
ΤT
        yl)amino]methyl]phenyl ester 854602-72-5P, Sulfamic acid
        2-chloro-4-[[N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]phenyl
        ester 854602-74-7P, Sulfamic acid 2-methoxy-4-[[N-(4-
        cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]phenyl ester
        854602-75-8P, Sulfamic acid 2,3,5,6-tetrafluoro-4-[[N-(4-
        cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]phenyl ester
        854602-78-1P, 4-[N-[(2,2-Dioxido-3,4-dihydro-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,2,3-benzoxathiazin-1,
        6-yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile 936575-32-5P
         , 4-[N-[(6-Chloropyridin-3-yl)methyl]-N-(1H-imidazol-1-
        yl)amino]benzonitrile 936575-33-6\mathbb{P}, 4-[[N-(4-Cyanophenyl)-N-(1H-
        imidazol-1-yl)amino]methyl]benzenesulfonamide 936575-35-8P,
        5-[[N-(4-Cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]-2-methoxybenzoic
        acid 936575-36-9P, 6-Chloro-N-(4-cyanophenyl)-N-(1H-imidazol-1-
        yl)nicotinamide 936575-37-0P, N-(1H-Imidazol-1-yl)-N-(4-
        cyanophenyl)-2-(4-fluorophenyl)acetamide 936575-47-2P,
        N-(4-Cyanophenyl)-N-(1H-imidazol-1-yl)-2-(6-hydroxybenzo[b]thien-3-
        yl)acetamide 936575-48-3P, 4-[N-(3-Amino-4-hydroxyphenylmethyl)-
        N-(1H-imidazol-1-yl)amino]benzonitrile 936575-57-4P
        936575-59-6P, Sulfamic acid 4-[2-[N-(4-cyanophenyl)-N-(1H-imidazol-
        1-yl)amino]ethoxy]phenyl ester 936575-60-9P, Sulfamic acid
        4-[[N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)carbamoyl]methyl]phenyl ester
        936575-61-0P 936575-62-1P, Sulfamic acid
        3-[(aminosulfonyl)amino]-4-[[N-(4-cyanophenyl)-N-(1H-imidazol-1-
        yl)amino]methyl]phenyl ester 936575-63-2P, 5-
         [(Aminosulfonyl)amino]-N-(4-cyanophenyl)-N-(1H-imidazol-1-
        yl)benzothiophene-2-carboxamide 936575-65-4P, Sulfamic acid
        3-[2-[N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)amino]-2-
        oxoethyl]benzo[b]thien-6-yl ester 936575-66-5P, Sulfamic acid
        3-[[N-(4-cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]benzo[b]thien-6-yl
        ester 936875-67-6P, Sulfamic acid 2-[[N-(4-cyanophenyl)-N-(1H-
        imidazol-1-yl)amino]methyl]benzo[b]thien-6-yl ester 936578-70-1P
         , 5-[[N-(4-Cyanophenyl)-N-(1H-imidazol-1-yl)amino]methyl]-2-hydroxybenzoic
        acid 936575-72-3P, 4-[N-[3-(Tosylamino)-4-hydroxybenzyl]-N-(1H-1)
        imidazol-1-yl)amino]benzonitrile 936575-74-5P,
         4-[N-[(2,2-Dioxido-3H-1,2,3-benzoxathiazol-5-yl)methyl]-N-(1H-imidazol-1-
        y1) amino] benzonitrile 936575-75-6P, 1-(4-Cyanopheny1)-1-(1H-Cyanopheny1)
        imidazol-1-yl)-3-phenylurea
        RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
         (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (Uses)
              (drug candidate; preparation of 1-N-Ph-amino-1H-imidazole derivs. as
              aromatase, steroid sulfatase, and carbonic anhydrase inhibitors and
              pharmaceutical compns. containing them)
RN
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CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]phenyl ester (CA INDEX NAME)

RN 854602-72-5 HCAPLUS

CN Sulfamic acid, 2-chloro-4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]phenyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 854602-74-7 HCAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2-methoxyphenyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ \text{MeO} & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ &$$

RN 854602-75-8 HCAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2,3,5,6-tetrafluorophenyl ester (CA INDEX NAME)

RN 854602-78-1 HCAPLUS

CN Benzonitrile, 4-[[(3,4-dihydro-2,2-dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-32-5 HCAPLUS

CN Benzonitrile, 4-[[(6-chloro-3-pyridinyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-33-6 HCAPLUS

CN Benzenesulfonamide, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]- (CA INDEX NAME)

RN 936575-35-8 HCAPLUS

CN Benzoic acid, 5-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2-methoxy-(CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\$$

RN 936575-36-9 HCAPLUS

CN 3-Pyridinecarboxamide, 6-chloro-N-(4-cyanophenyl)-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-37-0 HCAPLUS

CN Benzeneacetamide, N-(4-cyanophenyl)-4-fluoro-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-47-2 HCAPLUS

CN Benzo[b]thiophene-3-acetamide, N-(4-cyanophenyl)-6-hydroxy-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-48-3 HCAPLUS

CN Benzonitrile, 4-[[(3-amino-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 936575-57-4 HCAPLUS

CN Sulfamic acid, 2-bromo-4-[[(4-cyanophenyl)-1H-imidazol-1-

ylamino]methyl]phenyl ester, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

RN 936575-59-6 HCAPLUS
CN Sulfamic acid, 4-[2-[(4-cyanophenyl)-1H-imidazol-1-ylamino]ethoxy]phenyl ester (CA INDEX NAME)

RN 936575-60-9 HCAPLUS
CN Sulfamic acid, 4-[2-[(4-cyanophenyl)-1H-imidazol-1-ylamino]-2oxoethyl]phenyl ester (CA INDEX NAME)

RN 936575-61-0 HCAPLUS

CN Sulfamic acid, 4-[3-[(4-cyanophenyl)-1H-imidazol-1-ylamino]-3-oxopropyl]phenyl ester (CA INDEX NAME)

RN 936575-62-1 HCAPLUS

CN Sulfamic acid, 3-[(aminosulfonyl)amino]-4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]phenyl ester (CA INDEX NAME)

RN 936575-63-2 HCAPLUS

CN Benzo[b]thiophene-2-carboxamide, 5-[(aminosulfonyl)amino]-N-(4-cyanophenyl)-N-1H-imidazol-1-yl- (CA INDEX NAME)

RN 936575-65-4 HCAPLUS

CN Sulfamic acid, 3-[2-[(4-cyanophenyl)-1H-imidazol-1-ylamino]-2-oxoethyl]benzo[b]thien-6-yl ester (CA INDEX NAME)

RN 936575-66-5 HCAPLUS

CN Sulfamic acid, 3-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]benzo[b]thien-6-yl ester (CA INDEX NAME)

$$H_2N - \bigcup_{S=0}^{O} O \longrightarrow S \longrightarrow CH_2 - \bigcup_{N=N}^{CN} N$$

RN 936575-67-6 HCAPLUS

CN Sulfamic acid, 2-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]benzo[b]thien-6-yl ester (CA INDEX NAME)

$$H_2N$$
 $=$ 0 CH_2 $=$ N $=$ N

RN 936575-70-1 HCAPLUS

CN Benzoic acid, 5-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2-hydroxy-(CA INDEX NAME)

RN 936575-72-3 HCAPLUS

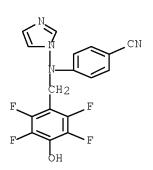
CN Benzenesulfonamide, N-[5-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2-hydroxyphenyl]-4-methyl- (CA INDEX NAME)

RN 936575-74-5 HCAPLUS

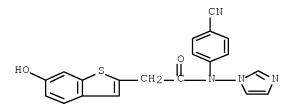
CN Benzonitrile, 4-[[(2,2-dioxido-3H-1,2,3-benzoxathiazol-5-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

$$N = N - CH_2$$

RN 936575-75-6 HCAPLUS CN Urea, N-(4-cyanophenyl)-N-1H-imidazol-1-yl-N'-phenyl- (CA INDEX NAME)



RN 936575-56-3 HCAPLUS
CN Benzo[b]thiophene-2-acetamide, N-(4-cyanophenyl)-6-hydroxy-N-1H-imidazol-1-yl- (CA INDEX NAME)



L44 ANSWER 4 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:1010090 HCAPLUS Full-text

DOCUMENT NUMBER: 145:376919

TITLE: Aminoethyl sulfonamide compounds and their

preparation, pharmaceutical composition,

structure-activity relationship, pharmacokinetics and

methods for the treatment of malaria and cancer

INVENTOR(S): Hamilton, Andrew; Buckner, Frederick; Glenn, Matthew;

Van Voorhis, Wesley

PATENT ASSIGNEE(S): Yale University, USA; University of South Florida;

University of Washington; Sebti, Said

PCT Int. Appl., 72pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PA'	TENT :	NO.			KIND		DATE			APPLICATION NO.						DATE			
					A2 20060928 A3 20070215				WO 2	006-									
WO	2006	006102159					2007	0215											
	W:	ΑE,	ΑG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,		
		KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,		
		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,		
		SG,	SK,	SL,	SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,		
		VN,	YU,	ZA,	ZM,	ZW													
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,		
		IS,	ΙT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,		
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,	GH,		
		GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,		
		KG,	KΖ,	MD,	RU,	ТJ,	TM												
PRIORIT	Y APP	LN.	INFO	.:						US 2005-663370P						P 20050317			
OTHER SOURCE(S): MARPAT 145:376919																			
ED En	tered	STN	: 2	9 Se	р 20	06													

AΒ Compds. of formula I according to the invention are useful in one or more aspects to inhibit farnesyl transferase, or to treat malaria, neoplasia, a hyperproliferative disease state or arthritis, including rheumatoid arthritis or osteoarthritis. Compds. of formula I wherein R1 is (un)substituted C3-12 hydrocarbyl, (un) substituted heterocyclyl and (un) substituted (hetero) aryl; R is alkyl, acyl, etc.; R5-R10 and RN are independently H, (un)substituted C1-12 hydrocarbyl, (un) substituted C5-12 cycloalkyl, (un) substituted heterocyclyl, (un) substituted (hetero) aryl, etc.; A is thioalkyl, azolylalkyl, carboxyalkyl, etc.; and their pharmaceutically acceptable salts thereof are claimed. Example compound II was prepared by amidation of N'-benzyl-N-(4-bromophenyl)-N-(3-methyl-2H- imidazol-4-ylmethyl)ethane-1,2-diamine with 1methylimidazolylsulfonyl acid derivative All the invention compds. were evaluated for their antimalaria and anticancer activity. The tested compds. showed good activity. The structure activity relationship and some pharmacokinetics are also reported.

IT 910910-59-7P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate and intermediate; preparation of aminoethyl sulfonamide compds. their structure-activity relationship, pharmacokinetics, and methods for the treatment of malaria and cancer)

RN 910910-59-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(4-piperidinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \text{-N-CH}_2 \text{-CH}_2 \\ \text{N} \end{array} \right) \begin{array}{c} \text{H} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \end{array} \right)$$

IT 865788-27-8P 865788-32-5P 865788-34-7P 910910-50-8P 910910-62-2P 910910-63-3P 910910-65-5P 910910-71-3P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of aminoethyl sulfonamide compds. their

structure-activity relationship, pharmacokinetics, and methods for the treatment of malaria and cancer)

RN 865788-27-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2\text{-Ph} \\ \text{CH}_2\text{-N-CH}_2\text{-CH}_2\text{-CH}_2\text{-N-S} \\ \text{Me} \end{array}$$

RN 865788-32-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(cyclohexylmethyl)-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{N}$$

RN 865788-34-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right) \begin{array}{c} \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right)$$

RN 910910-50-8 HCAPLUS

CN 2-Pyridinesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 910910-62-2 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 910910-63-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[1-(2-pyrimidinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{Me} \\ \text{O} \\ \text{S} \\ \text{O} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{N}$$

RN 910910-65-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(4-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{Me} \\ \text{N} \end{array}$$

RN 910910-71-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-([1,1'-biphenyl]-3-ylmethyl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} & \text{Ph} \\ \text{Me} & \text{CH}_2 & \text{O} \\ \text{N} & \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array}$$

IT 865788-30-3P 865788-31-4P 865788-33-6P 865788-35-8P 910910-49-5P 910910-51-9P 910910-52-0P 910910-53-1P 910910-54-2P 910910-55-3P 910910-56-4P 910910-57-5P 910910-58-6P 910910-60-0P 910910-61-1P 910910-64-4P 910910-66-6P 910910-67-7P 910910-68-8P 910910-69-9P 910910-70-2P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aminoethyl sulfonamide compds. their structure-activity relationship, pharmacokinetics, and methods for the treatment of malaria and cancer)

RN 865788-30-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-31-4 HCAPLUS

CN 1-Naphthalenesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-5-(dimethylamino)-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-33-6 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2 - \text{C} - \text{NHBu-t} \\ \text{N} \\ \text{N} \\ \text{Me} \end{array}$$

RN 865788-35-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(2-methylphenyl)methyl]- (CA INDEX NAME)

RN 910910-49-5 HCAPLUS

CN 2-Thiophenesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \end{array} \begin{array}{c} \text{CH}_2 - \text{Ph} \\ \text{O} \\ \text{N} \end{array} \begin{array}{c} \text{CH}_2 - \text{Ph} \\ \text{O} \\ \text{O} \end{array} \begin{array}{c} \text{S} \\ \text{S} \end{array}$$

RN 910910-51-9 HCAPLUS

CN 8-Quinolinesulfonamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 910910-52-0 HCAPLUS

CN Acetamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

$$CH_2-Ph$$
 CH_2-CH_2-N-Ac
 CH_2-CH_2-N-Ac
 CH_2-CH_2-N-Ac

RN 910910-53-1 HCAPLUS

CN Propanamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-

y1)methy1]amino]ethy1]-2-methy1-N-(phenylmethy1)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{Ph} & \text{O} \\ \text{CH}_2-\text{CH}_2-\text{N} & \text{CN} \\ \end{array}$$

RN 910910-54-2 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-2-propen-1-yl- (CA INDEX NAME)

$$\begin{array}{c|c} CN & CH_2-CH \longrightarrow CH_2 \\ \hline \\ N & CH_2-N-CH_2-CH_2-N-S \\ \hline \\ Me & Me \end{array}$$

RN 910910-55-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(2-methyl-2-propen-1-yl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{C} - \text{Me} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{Me} \end{array}$$

RN 910910-56-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-(2-bromo-2-propen-1-yl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-(CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{C} - \text{Br} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{Me} \end{array}$$

RN 910910-57-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[2-(1H-pyrrol-1-yl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2 \\
\text{N} \\
\text{CH}_2 \\
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{CH}_2 \\
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2
\end{array}$$

RN 910910-58-6 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(tetrahydro-2H-pyran-4-yl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right)$$

RN 910910-60-0 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(1-acetyl-4-piperidinyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{Me} \\ \text{N} \end{array}$$

RN 910910-61-1 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[1-(2-methyl-1-oxopropyl)-4-piperidinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} & & & \\ & &$$

RN 910910-64-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(3-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array}$$

RN 910910-66-6 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(2-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \stackrel{\text{Me}}{\underset{\text{N}}{\longrightarrow}} \text{CH}_2 - \text{NH}_2 - \text{CH}_2 - \text{CH}_2 - \text{NH}_2 \\ \stackrel{\text{CH}_2}{\underset{\text{N}}{\longrightarrow}} \text{CH}_2 - \text{NH}_2 - \text{CH}_2 - \text{NH}_2 \\ \end{array}$$

RN 910910-67-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(3-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right)$$

RN 910910-68-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(4-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 \text{ CH}_2 \text{ CH}_2 \text{ CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{Me} \\ \text{CH}_2 \text{ CH}_2 \\ \text{N} \end{array}$$

RN 910910-69-9 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(3-cyanophenyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-(CAINDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 - \text{N-CH}_2 - \text{CH}_2 - \text{N-CH}_2 \\ \end{array}$$

RN 910910-70-2 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(4-cyanophenyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array}$$

IT 865788-39-2P 865788-42-7P 865788-43-8P 865788-44-9P 865788-45-0P 865788-46-1P 910910-72-4P 910910-73-5P 910910-82-6P 910910-84-8P 910910-86-0P 910910-87-1P 910910-88-2P 910910-89-3P 910910-93-9P 910910-94-0P 910910-95-1P 910910-96-2P 910910-97-3P 910910-98-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of aminoethyl sulfonamide compds. their structure-activity relationship, pharmacokinetics, and methods for the treatment of malaria and cancer)

RN 865788-39-2 HCAPLUS

CN Carbamic acid, [2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 865788-42-7 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(phenylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 865788-43-8 HCAPLUS

CN Benzonitrile, 4-[[2-[(cyclohexylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

RN 865788-44-9 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

RN 865788-45-0 HCAPLUS

CN Benzonitrile, 4-[[2-[([1,1'-biphenyl]-4-ylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \stackrel{\text{Me}}{\longrightarrow} \\ \stackrel{\text{N}}{\longrightarrow} \\ \stackrel{\text{CH}_2-\text{N}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2}{\longrightarrow} \end{array}$$

RN 865788-46-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(2-methyl-1H-imidazol-5-yl)methyl]]

methylphenyl)methyl]amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 910910-72-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[3-(1H-pyrrol-1-yl)phenyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array}$$

RN 910910-73-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[4-(1H-pyrrol-1-yl)phenyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \end{array} \end{array} \begin{array}{c} \\ \\ \\ \end{array} \begin{array}{c} \\ \\ \end{array} \begin{array}{$$

RN 910910-82-6 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-(2-propen-1-ylamino)ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} & \text{CH}_2\text{-CH}_2\text{-NH-CH}_2\text{-CH}_2\text{-CH}_2\\ \text{N} & \text{CH}_2\text{-NH-CH}_2\text{$$

RN 910910-84-8 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(2-methyl-2-propen-1-yl)amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{Me} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{C} - \text{Me} \\ \text{CH}_2 - \text{C} \\ \text{C} - \text{Me} \\ \text{C} - \text{C} \\ \text{C} - \text{C}$$

RN 910910-86-0 HCAPLUS

CN Benzonitrile, 4-[[2-[(2-bromo-2-propen-1-yl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \overset{\text{CH}_2}{\text{C-Br}} \\ \text{CN} \end{array}$$

RN 910910-87-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[2-(1H-pyrrol-1-yl)ethyl]amino]- (CA INDEX NAME)

RN 910910-88-2 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(tetrahydro-2H-pyran-4-yl)methyl]amino]- (CA INDEX NAME)

RN 910910-89-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(3-methylphenyl)methyl]amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{Me}
\end{array}$$

RN 910910-90-6 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(4-methylphenyl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 910910-91-7 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(2-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-92-8 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(3-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-93-9 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(4-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-94-0 HCAPLUS

CN Benzonitrile, 3-[[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]amino]methyl]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CN}
\end{array}$$

RN 910910-95-1 HCAPLUS

CN Benzonitrile, 4-[[2-[[(4-cyanophenyl)methyl]amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CN} \\
\text{CN}
\end{array}$$

RN 910910-96-2 HCAPLUS

CN Benzonitrile, 4-[[2-[([1,1'-biphenyl]-3-ylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Ph} \\
\text{CN}
\end{array}$$

RN 910910-97-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[[3-(1H-pyrrol-1-yl)phenyl]methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{N}
\end{array}$$

RN 910910-98-4 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[[4-(1H-pyrrol-1-yl)phenyl]methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

IT 910911-00-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of aminoethyl sulfonamide compds. their structure-activity relationship, pharmacokinetics, and methods for the treatment of malaria and cancer)

RN 910911-00-1 HCAPLUS

CN Benzonitrile, 4-[(2-aminoethyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 910910-99-5 CMF C14 H17 N5

$$\begin{array}{c} \text{Me} & \text{CH}_2 - \text{CH}_2 - \text{NH}_2 \\ \text{N} & \text{CH}_2 - \text{N} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L44 ANSWER 5 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:655773 HCAPLUS Full-text

DOCUMENT NUMBER: 145:124468

TITLE: Preparation of 3,4-substituted piperidine compounds as

renin inhibitors

INVENTOR(S): Breitenstein, Werner; Ehara, Takeru; Ehrhardt, Claus;

Grosche, Philipp; Hitomi, Yuko; Iwaki, Yuki; Kanazawa, Takanori; Konishi, Kazuhide; Maibaum, Juergen Klaus; Masuya, Keiichi; Nihonyanagi, Atsuko; Ostermann, Nils;

Suzuki, Masaki; Toyao, Atsushi; Yokokawa, Fumiaki

PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma GmbH

SOURCE: PCT Int. Appl., 633 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	KIND DATE				APPLICATION NO.						DATE							
WO :	WO 2006069788					A1		20060706		WO 2005-EP14102					20051228			
	W:	ΑE,	AG,	AL,	ΑM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KN,	KP,	KR,	
		KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	
		MZ,	NA,	NG,	NΙ,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	
		SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	
		VN,	YU,	ZA,	ZM,	ZW												
	RW:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	
		IS,	ΙΤ,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	${ m ML}$,	MR,	ΝE,	SN,	TD,	ΤG,	BW,	GH,	
		GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,	ΑZ,	BY,	
		KG,	KΖ,	MD,	RU,	ТJ,	TM											
AU :	AU 2005321475				A1		2006	0706	AU 2005-321475						20051228			
CA :	CA 2587348				A1	A1 20060706				CA 2005-2587348					20051228			
EP :	2 1833816				A1	20070919				EP 2005-820552					20051228			
	R:	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	
		IS,	,	,	,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR		
	CN 101094848					20071226			1	CN 2005-80045028					20051228			
JP :	JP 2008526701								1	JP 2007-548756					20051228			
									IN 2007-DN3696									
MX 200708078				А	20070724				MX 2007-8078					20070629				
KR :	KR 2007091174				А	20070907				KR 2007-715024					20070629			
.IORITY	ORITY APPLN. INFO.:									GB 2004-28526								
					•	WO 2	005-1	EP14:	102	1	W 2	0051	228					

OTHER SOURCE(S): MARPAT 145:124468

ED Entered STN: 07 Jul 2006

GI

$$\mathbb{R}^{2} \xrightarrow{\mathbb{N}}_{\mathbb{T}} \mathbb{R}^{1} \mathbb{W}$$

AB The title compds. I [R1 = H, alkyl, aryl, etc.; R2 = alkyl, aryl, heterocyclyl, etc.; W = substituted Ph, pyridyl, etc.; T = methylene or carbonyl; R11 = H, OH, halo, etc.] were prepared and formulated for use in the diagnostic and therapeutic treatment of a warm-blooded animal, especially for the treatment of a disease (or disorder) that depends on activity of renin. E.g., a multi-step synthesis of II, starting from 4-trifluoromethanesulfonyloxy-5,6-dihydro-2H-pyridine-1,3-dicarboxylic acid 1-tert-Bu ester 3-Me ester and 3-biphenylboronic acid, was given. Compds. I preferably show IC50 values in the range from 1 nM to 5 μ M in recombinant human renin assay (no specific data given).

IT 897945-83-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3,4-substituted piperidine compds. as renin inhibitors) RN 897945-83-4 HCAPLUS

CN 3-Piperidinecarboxamide, 4-[1,1'-biphenyl]-3-yl-N-[4-cyano-3-(3-methoxypropoxy)phenyl]-N-cyclopropyl-, (3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

IT 897955-95-2P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 3,4-substituted piperidine compds. as renin inhibitors) 897955-95-2 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[1,1'-biphenyl]-3-yl-3-[[[4-cyano-3-(3-methoxypropoxy)phenyl]cyclopropylamino]carbonyl]-, 1,1-dimethylethyl ester, (3R,4S)-rel- (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 6 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:852846 HCAPLUS Full-text

DOCUMENT NUMBER: 145:410021

TITLE: Structurally Simple, Potent, Plasmodium Selective

Farnesyltransferase Inhibitors That Arrest the Growth

of Malaria Parasites

AUTHOR(S): Glenn, Matthew P.; Chang, Sung-Youn; Horney, Carrie;

Rivas, Kasey; Yokoyama, Kohei; Pusateri, Erin E.; Fletcher, Steven; Cummings, Christopher G.; Buckner, Frederick S.; Pendyala, Prakash R.; Chakrabarti,

Debopam; Sebti, Saied M.; Gelb, Michael; Van Voorhis,

Wesley C.; Hamilton, Andrew D.

CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,

CT, 06511, USA

SOURCE: Journal of Medicinal Chemistry (2006), 49(19),

5710-5727

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:410021

ED Entered STN: 25 Aug 2006

AB Third world nations require immediate access to inexpensive therapeutics to counter the high mortality inflicted by malaria. Here, the authors report a new class of antimalarial protein farnesyltransferase (PFT) inhibitors, designed with specific emphasis on simple mol. architecture, to facilitate easy access to therapies based on this recently validated antimalarial target. This novel series of compds. represents the first Plasmodium falciparum selective PFT inhibitors reported (up to 145-fold selectivity), with lead inhibitors displaying excellent in vitro activity (IC50 < 1 nM) and toxicity to cultured parasites at low concns. (ED50 < 100 nM). Initial studies of absorption, metabolism, and oral bioavailability are reported.

IT 865788-27-8P 865788-32-5P 865788-34-7P 865788-35-8P 910910-50-8P 910910-62-2P 910910-63-3P 910910-66-6P 910910-73-5P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structurally simple, potent, Plasmodium selective farnesyltransferase inhibitors that arrest the growth of malaria parasites)

RN 865788-27-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-

y1)methy1]amino]ethy1]-1-methy1-N-(phenylmethy1)- (CA INDEX NAME)

$$CH_2$$
—Ph

 CH_2 —Ph

 CH_2 —Ph

 CH_2 —Ph

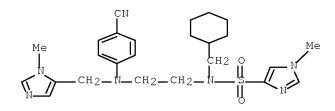
 CH_2 —Ph

 CH_2 —Ph

 CH_2 —Ph

RN 865788-32-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(cyclohexylmethyl)-1-methyl- (CA INDEX NAME)



RN 865788-34-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array} \right) \begin{array}{c} \text{Ph} \\ \text{CH}_2 \\ \text{O} \\ \text{N} \end{array} \right)$$

RN 865788-35-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(2-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array}$$

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \end{array}$$

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array}$$

RN 910910-50-8 HCAPLUS

CN 2-Pyridinesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

$$\stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{N}$$

RN 910910-62-2 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

RN 910910-63-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[1-(2-pyrimidinyl)-4-piperidinyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{Me} \\ \text{O} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} - \text{CH}_2 \end{array}$$

RN 910910-66-6 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(2-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array} \right) \begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array}$$

RN 910910-73-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[4-(1H-pyrrol-1-yl)phenyl]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array}$$

IT 865788-30-3P 865788-31-4P 865788-33-6P 910910-49-5P 910910-51-9P 910910-52-0P 910910-53-1P 910910-54-2P 910910-55-3P 910910-56-4P 910910-57-5P 910910-58-6P 910910-59-7P 910910-60-0P 910910-61-1P 910910-64-4P 910910-65-5P 910910-67-7P 910910-68-8P 910910-69-9P 910910-70-2P 910910-71-3P 910910-72-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(structurally simple, potent, Plasmodium selective farnesyltransferase inhibitors that arrest the growth of malaria parasites)

RN 865788-30-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-31-4 HCAPLUS

CN 1-Naphthalenesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-5-(dimethylamino)-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-33-6 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

RN 910910-49-5 HCAPLUS

CN 2-Thiophenesulfonamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{N} \\ \text{S} \\ \text{$$

RN 910910-51-9 HCAPLUS

CN 8-Quinolinesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 910910-52-0 HCAPLUS

CN Acetamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

$$CH_2-Ph$$
 CH_2-CH_2-N-Ac
 CH_2-CH_2-N-Ac
 CH_2-CH_2-N-Ac

RN

CN Propanamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-2-methyl-N-(phenylmethyl)- (CA INDEX NAME)

RN 910910-54-2 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-2-propen-1-yl- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2\text{-CH} \longrightarrow \text{CH}_2\\ \text{CH}_2\text{--}\text{CH}_2\text{---}\text{CH}_2\text{---}\text{CH}_2\\ \text{Me} \end{array}$$

RN 910910-55-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(2-methyl-2-propen-1-yl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{C}_{-\text{Me}} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{Me} \end{array}$$

RN 910910-56-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-(2-bromo-2-propen-1-yl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{Me} \end{array}$$

RN 910910-57-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[2-(1H-pyrrol-1-yl)ethyl]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2 \\
\text{N} \\
\text{CH}_2 \\
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{CH}_2 \\
\text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2
\end{array}$$

RN 910910-58-6 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(tetrahydro-2H-pyran-4-yl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right) \\ \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{N}$$

RN 910910-59-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(4-piperidinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{N}$$

RN 910910-60-0 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(1-acetyl-4-piperidinyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \begin{array}{c} \text{Me} \\ \text{N} \end{array}$$

RN 910910-61-1 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[1-(2-methyl-1-oxopropyl)-4-piperidinyl]methyl]- (CA INDEX NAME)

RN 910910-64-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(3-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{N} \\$$

RN 910910-65-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(4-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right) \xrightarrow{\text{Me}} \\ \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\$$

RN 910910-67-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(3-pyridinylmethyl)- (CA INDEX NAME)

RN 910910-68-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(4-pyridinylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{N} \end{array}$$

RN 910910-69-9 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(3-cyanophenyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-(CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 - \text{N-CH}_2 - \text{CH}_2 - \text{N-S} \\ \end{array}$$

RN 910910-70-2 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[(4-cyanophenyl)methyl]-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-(CAINDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2 \\$$

RN 910910-71-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-([1,1'-biphenyl]-3-ylmethyl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} & \text{Ph} \\ \text{CH}_2 & \text{O} \\ \text{N} \end{array}$$

RN 910910-72-4 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[[3-(1H-pyrrol-1-yl)phenyl]methyl]- (CA

INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2 - \text{N-CH}_2 - \text{CH}_2 - \text{N-CH}_2 \\ \end{array}$$

IT 910911-00-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (structurally simple, potent, Plasmodium selective farnesyltransferase inhibitors that arrest the growth of malaria parasites)
RN 910911-00-1 HCAPLUS
CN Benzonitrile, 4-[(2-aminoethyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]-,
 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

CRN 910910-99-5
CMF C14 H17 N5

CM 2

CRN 76-05-1

CMF C2 H F3 O2

IT 865788-39-2P 865788-42-7P 865788-43-8P 865788-44-9P 865788-45-0P 865788-46-1P 910910-82-6P 910910-84-8P 910910-89-3P 910910-90-6P 910910-91-7P 910910-92-8P 910910-93-9P 910910-94-0P 910910-95-1P 910910-96-2P 910910-97-3P 910910-98-4P

912482-46-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(structurally simple, potent, Plasmodium selective farnesyltransferase inhibitors that arrest the growth of malaria parasites)

RN 865788-39-2 HCAPLUS

CN Carbamic acid, [2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 865788-42-7 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(phenylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 865788-43-8 HCAPLUS

CN Benzonitrile, 4-[[2-[(cyclohexylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

RN 865788-44-9 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NH} \\ \text{NH} - \text{CH}_2 - \text{NH} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NH} \\ \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} \\ \text{CH}_2 - \text{NH} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} \\ \text{CH}_2 - \text{NH} \\$$

RN 865788-45-0 HCAPLUS

CN Benzonitrile, 4-[[2-[([1,1'-biphenyl]-4-ylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 865788-46-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(2-methylphenyl)methyl]amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 910910-82-6 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-(2-propen-1-ylamino)ethyl]amino]- (CA INDEX NAME)

RN 910910-84-8 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(2-methyl-2-propen-1-yl)amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{Me} \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{C} - \text{Me} \\ \text{CH}_2 - \text{C} \\ \text{C} - \text{C} \\ \text$$

RN 910910-86-0 HCAPLUS

CN Benzonitrile, 4-[[2-[(2-bromo-2-propen-1-yl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 \\ \text{Me} \\ \text{N} \end{array} \quad \begin{array}{c} \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C-Br} \\ \text{CN} \end{array}$$

RN 910910-87-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[2-(1H-pyrrol-1-yl)ethyl]amino]- (CA INDEX NAME)

RN 910910-88-2 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(tetrahydro-2H-pyran-4-yl)methyl]amino]- (CA INDEX NAME)

RN 910910-89-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(3-methylphenyl)methyl]amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{Me}
\end{array}$$

RN 910910-90-6 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(4-methylphenyl)methyl]amino]ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{CH}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{NH} - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{CH}_2 \\ \\ \stackrel{\text{Me}}{\underset{N}{\longrightarrow}} \text{CH}_2 - \text{$$

RN 910910-91-7 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(2-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-92-8 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(3-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-93-9 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(4-pyridinylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 910910-94-0 HCAPLUS

CN Benzonitrile, 3-[[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]amino]methyl]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CN}
\end{array}$$

RN 910910-95-1 HCAPLUS

CN Benzonitrile, 4-[[2-[[(4-cyanophenyl)methyl]amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 910910-96-2 HCAPLUS

CN Benzonitrile, 4-[[2-[([1,1'-biphenyl]-3-ylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Ph} \\
\text{CN}
\end{array}$$

RN 910910-97-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[[3-(1H-pyrrol-1-yl)phenyl]methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{N}
\end{array}$$

RN 910910-98-4 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[[4-(1H-pyrrol-1-yl)phenyl]methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\stackrel{\text{Me}}{\underset{\text{N}}{\longrightarrow}} \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

RN 912482-46-3 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \overset{\text{CN}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{NH}_2 - \text{CH}_2 - \text{NH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 \\ & \overset{\text{CH}}{\underset{\text{Me}}{\bigvee}} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\$$

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 7 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:1042201 HCAPLUS Full-text

DOCUMENT NUMBER: 143:326203

TITLE: Arylamines as androgen receptor modulators, their preparation, pharmaceutical compositions, and use in

therapy

INVENTOR(S): Zhi, Lin; Higuchi, Robert I.; Kallel, E. Adam; Van

Oeveren, Cornelis Arjan; Chen, Jyun-Hung; Ruppar, Daniel A.; Pedram, Bijan; Lau, Thomas Lot Stevens;

Miller, Todd

PATENT ASSIGNEE(S): Ligand Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GΙ

	PATENT NO.						D	DATE APPLICATION NO.						DATE				
	WO 2005090282			A1 20050929			WO 2005-US7867						20050311					
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,
			NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,
			SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙT,	LT,	LU,	MC,	NL,	PL,	PT,
			RO,	SE,	SI,	SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
			MR,	ΝE,	SN,	TD,	ΤG											
	US	2007	0254	875		A1		2007	1101		US 2	007-	5901	19		2	0070	611
PRIO	PRIORITY APPLN. INFO.:										US 2	004-	5526	90P		P 2	0040	312
											WO 2	005-	US78	67	,	W 2	0050	311
OTHE	OTHER SOURCE(S): CASREACT 143:326203; MARPAT 143:326203																	
ED	ED Entered STN: 29 Sep 2005																	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The invention relates to a group of amines, e.g., I, which act as modulators AB of androgen receptors and/or androgen receptor binding agents. In compds. I, R1 and R2 are independently selected from H, F, Cl, Br, I, OH, (un)substituted C1-4 alkoxy, etc.; R3, R4, and R5 are independently selected from H, F, C1, OH, (un) substituted C1-4 alkoxy, (un) substituted C1-4 alkyl, and (un) substituted C1-4 haloalkyl; R6 and R7 are independently selected from H, (un) substituted C1-6 alkyl, (un) substituted C1-6 haloalkyl, (un) substituted C1-6 heteroalkyl, (un)substituted C2-6 alkynyl, and (un)substituted C2-6 alkenyl, or R6 and R7 together form a carbonyl; R9 is selected from H, (un)substituted C1-8 alkyl, (un)substituted C2-8 alkenyl, (un)substituted C1-8 haloalkyl, (un)substituted aryl, (un)substituted heteroaryl, etc.; R10 is selected from H, (un)substituted C1-6 alkyl, (un)substituted C1-6 haloalkyl, (un)substituted C1-6 heteroalkyl, (un)substituted C2-6 alkynyl, and (un)substituted C2-6 alkenyl; R12 and R13 are independently selected from H, F, Cl, OH, (un) substituted C1-4 alkoxy, (un) substituted amino, (un) substituted C1-6 alkyl, etc.; Z is O, S, (un)substituted C, or (un)substituted N; and n is 0-2; provided that if R1 is NO2 and R3 is F, then Z is not O; including pharmaceutically acceptable salts, esters, amides or prodrugs thereof. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. containing compds. of the invention along with a pharmaceutically acceptable carrier, as well as to the use of the compns. for treating various conditions. 3-(Trifluoromethyl)-4-nitrobromobenzene underwent palladium-mediated coupling with chiral pyrrolidinone II followed by reduction to the corresponding pyrrolidine, and desilylation to give alc. III. Oxidation of III to the corresponding aldehyde was followed by addition of

TMSCF3 to give IV along with its separable (R,R)-diastereomer. Some of the compds. of the invention act as androgen receptor agonists, others as androgen receptor antagonists, androgen receptor partial agonists, or tissue-specific modulators (no data).

IT 821777-55-3P, 4-[Bis(2,2,2-trifluoroethyl)amino]-2-

(trifluoromethyl)benzonitrile

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of arylamines as androgen receptor modulators) 821777-55-3 HCAPLUS

CN Benzonitrile, 4-[bis(2,2,2-trifluoroethyl)amino]-2-(trifluoromethyl)- (CA INDEX NAME)

RN

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 8 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:116451 HCAPLUS Full-text

DOCUMENT NUMBER: 142:191223

TITLE: Styrene derivatives as tyrosine kinase inhibitors, their preparation, their prodrugs, pharmaceuticals

containing them, combination therapy using them, and

use of them in manufacture of tyrosine kinase

inhibitors and antitumor agents

INVENTOR(S): Tasaka, Akihiro; Taniguchi, Takahiko; Tsujimoto,

Saori; Naito, Kenichiro

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 82 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ----_____ _____ _____ _____ JP 2005035944 JP 2003-275675 A 20050210 20030716 PRIORITY APPLN. INFO.: JP 2003-275675 20030716

OTHER SOURCE(S): MARPAT 142:191223

ED Entered STN: 10 Feb 2005

GΙ

$$\begin{array}{c|c}
R^1 & R^5 & R^7 \\
R^2 & R^3 & R^4 & R^9
\end{array}$$

The derivs. I [n = 1, 2; Y = 0, S; R1 = halo, C1-2 (halo)alkyl; R2, R3 = H,AΒ halo, C1-2 (halo)alkyl; R4 = H, OH, C1-4 (halo)alkyl; R5 = halo, cyano, OH, C1-6 (halo)alkyl, C1-6 hydroxyalkoxy, C1-6 haloalkoxy, carboxy, C1-6 alkoxycarbonyl; R6-R8 = H, any group given for R5; R9 = triazolylalkyl Q, imidazolylalkyl Q1 (m = 2-5; R10 = C1-6 alkyl which may be substituted with 1-3 OH)] or their salts, useful for prevention/treatment of cancers, are prepared by reacting styryl(oxazoles or thiazoles) II (R1-R4, n, Y = same as above; X = leaving group) or their salts with phenols III (R5-R9 = same as above) or their salts. Also claimed are prodrugs of I, pharmaceutical compns. containing I (salts) or their prodrugs, drugs combining I (salts) or their prodrugs with antitumor agents or hormones such as leuprorelin, method for inhibition of tyrosine kinase or prevention/treatment of cancers by administering I (salts) or their prodrugs to mammals, and use of I (salts) or their prodrugs in manufacture of tyrosine kinase inhibitors and antitumor agents. Administration of I (salts) or their prodrugs may be performed prior to surgery, radiotherapy, gene therapy, hyperthermia, cryotherapy, and/or laser cauterization. Thus, [1-[4-[4-[2-[(E)-2-(4-bromo-2-(4-bromfluorophenyl)ethenyl]-1,3-oxazol-4- yl]methoxy]-2-methylphenyl]butyl]-1Himidazol-2-yl]methanol (IV; preparation given) inhibited growth of human BT-474 breast cancer cell at IC50 <0.05 μ M. Tablets containing IV were also formulated.

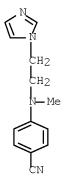
IT 568594-05-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocycle-containing styrene derivs. as tyrosine kinase inhibitors for prevention/treatment of cancers, etc.)

RN 568594-05-8 HCAPLUS

CN Benzonitrile, 4-[[2-(1H-imidazol-1-yl)ethyl]methylamino]- (CA INDEX NAME)



L44 ANSWER 9 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:539693 HCAPLUS Full-text

DOCUMENT NUMBER: 143:59983

TITLE: Preparation of phenylaminoimidazoles as aromatase

and/or steroid sulfatase and/or carbonic anhydrase

inhibitors.

INVENTOR(S): Lafay, Jean; Rondot, Benoit; Bonnet, Paule; Clerc,

Thierry; Shields, Jacqueline; Duc, Igor; Duranti, Eric; Puccio, François; Blot, Christian; Maillos,

Philippe

PATENT ASSIGNEE(S): Laboratoire Theramex, Monaco

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.				KIND DATE				APPLICATION NO.					DATE					
EP	1544	195			A1		2005	0622		EP 2	003-	2931	52		2	0031	215	
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	SI,	LT,	LV,	FΙ,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK		
ΑU	2004	2992	86		A1		2005	0630		AU 2004-299286					20041215			
CA	2549	603			A1		2005	0630	CA 2004-2549603						20041215			
WO	2005	0588	42		A1		2005	0630		WO 2004-EP14847					20041215			
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AΖ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	KΖ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,	
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,	
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	
		MR,	ΝE,	SN,	TD,	ΤG												
EP	1694	650			A1		2006	0830	EP 2004-804432						20041215			
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	SI,	LT,	FΙ,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	IS			
CN	CN 1890221			Α		2007	0103		CN 2004-80036357					20041215				
BR	2004	0174	07		Α		2007	0403		BR 2	004-	1740	7		20041215			
JP	P 2007515420			Τ		2007	0614		JP 2006-544394						20041215			

NO 2006002710	Α	20060630	ИО	2006-2710		20060612
IN 2006DN03428	A	20070420	IN	2006-DN3428		20060614
MX 2006PA06837	A	20060904	MX	2006-PA6837		20060615
US 20070112009	A1	20070517	US	2006-582778		20060817
PRIORITY APPLN. INFO.:			EP	2003-293152	A	20031215
			EP	2004-292681	A	20041112
			WO	2004-EP14847	W	20041215

OTHER SOURCE(S): CASREACT 143:59983; MARPAT 143:59983

ED Entered STN: 23 Jun 2005

GΙ

$$\begin{array}{c}
\mathbb{R}^{1} \\
\mathbb{R}^{2} \\
\mathbb{R}^{3} \\
\mathbb{R}^{6}
\end{array}$$

$$\begin{array}{c}
\mathbb{R}^{2} \\
\mathbb{R}^{2} \\
\mathbb{R}^{2} \\
\mathbb{R}^{4} \\
\mathbb{R}^{5} \\
\mathbb{R}^{n}$$

Title compds. [I; R1, R2 = H, alkyl, cycloalkyl; R1R2 = atoms to form a 5-7 membered (unsatd.) carbocyclyl; n = 0-2; 1 of R3, R4 = OH, NO2, NR7R8, OSO2NR7R8, NR7SO2NR7R8; the other of R3, R4 = H, OH, cyano, halo, NO2, alkyl, alkoxy, CF3, alkylthio, alkylsulfonyl, acyl, alkoxycarbonyl, carboxamido, NR7R8, OSO2NR7R8, NR7SO2NR7R8; R7, R8 = H, alkyl, cycloalkyl; m = 1-4; R5, R6 = OH, cyano, halo, NO2, alkyl, alkoxy, CF3, alkylthio, alkylsulfonyl, acyl, alkoxycarbonyl, carboxamido, R7R8, OSO2NR7R8, NR7SO2NR7R8; R4RR5 = atoms to form a benzoxathiazine dioxide or dihydrobenzoxathiazine dioxide ring; R3R6 = atoms to form a benzofuryl, N-methylbenzotriazole ring], were prepared Thus, a mixture of 4-hydroxybenzyl bromide, 4-[N-(1H-imidazol-1-yl)amino]benzonitrile (preparation given), and K2CO3 were stirred together for 2 h in THF to give 41% 4-[N-(4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile. The latter inhibited human aromatase with IC50 = 0.16 nM.

IT 854602-76-9P, 4-[N-[(2,2-Dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of phenylaminoimidazoles as aromatase and/or steroid sulfatase and/or carbonic anhydrase inhibitors)

RN 854602-76-9 HCAPLUS

CN Benzonitrile, 4-[((2,2-dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

ΙT 854602-62-3P, 4-[N-(4-Hydroxyphenylmethyl)-N-(1H-imidazol-1-M-imidyl)amino]benzonitrile 854602-63-4P, 4-[N-(3-Chloro-4hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-64-5P, 4-[N-(3-Bromo-4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-65-6P, 4-[N-(4-Hydroxy-3-1)]methoxyphenylmethyl)-N-(1H-imidazol-1-yl)amino|benzonitrile 854602-66-7P, 4-[N-(2,3,5,6-Tetrafluoro-4-hydroxyphenylmethyl)-N-(1H-imidazol-1-yl)amino]benzonitrile 854602-67-8P, 4-[N-(3-Formyl-4-hydroxyphenylmethyl)-N-(1H-imidazol-1yl)amino]benzonitrile 854602-71-4P 854602-72-5P 854602-73-6P 854602-74-7P 854602-75-8P 854602-78-1P, 4-[N-[(2,2-Dioxido-3,4-dihydro-1,2,3-benzoxathiazin-6-yl)methyl]-N-(1H-imidazol-1-yl)amino]benzonitrile RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of phenylaminoimidazoles as aromatase and/or steroid sulfatase and/or carbonic anhydrase inhibitors) 854602-62-3 HCAPLUS RNCN Benzonitrile, 4-[[(4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-63-4 HCAPLUS
CN Benzonitrile, 4-[[(3-chloro-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino](CA INDEX NAME)

RN 854602-64-5 HCAPLUS

CN Benzonitrile, 4-[[(3-bromo-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-65-6 HCAPLUS

CN Benzonitrile, 4-[[(4-hydroxy-3-methoxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ CH_2 \\ CN \\ \end{array}$$

RN 854602-66-7 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[(2,3,5,6-tetrafluoro-4-hydroxyphenyl)methyl]amino]- (CA INDEX NAME)

CN Benzonitrile, 4-[[(3-formyl-4-hydroxyphenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-71-4 HCAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]phenyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 854602-72-5 HCAPLUS

CN Sulfamic acid, 2-chloro-4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]phenyl ester (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ CH_2 \end{array} \\ CN \\ H_2N \\ \end{array}$$

RN 854602-73-6 HCAPLUS

CN Benzonitrile, 4-[[[4-[(aminosulfonyl)oxy]-3-bromophenyl]methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 854602-74-7 HCAPLUS

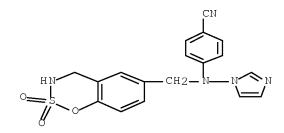
CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2-methoxyphenyl ester (CA INDEX NAME)

RN 854602-75-8 HCAPLUS

CN Sulfamic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-2,3,5,6-tetrafluorophenyl ester (CA INDEX NAME)

RN 854602-78-1 HCAPLUS

CN Benzonitrile, 4-[[(3,4-dihydro-2,2-dioxido-1,2,3-benzoxathiazin-6-yl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 10 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:954488 HCAPLUS Full-text

DOCUMENT NUMBER: 143:338963

TITLE: Structurally simple farnesyltransferase inhibitors

arrest the growth of malaria parasites

AUTHOR(S): Glenn, Matthew P.; Chang, Sung-Youn; Hucke, Oliver; Verlinde, Christophe L. M. J.; Rivas, Kasey; Horney,

Carrie; Yokoyama, Kohei; Buckner, Frederick S.; Pendyala, Prakash R.; Chakrabarti, Debopam; Gelb,

Michael; Van Voorhis, Wesley C.; Sebti, Said M.;

Hamilton, Andrew D.

CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,

CT, 06511, USA

SOURCE: Angewandte Chemie, International Edition (2005),

44(31), 4903-4906

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:338963

ED Entered STN: 01 Sep 2005

AB Antimalarial compds.: Structurally simple acyclic inhibitors of protein farnesyltransferase (active-site model shown) from the malaria parasite

Plasmodium falciparum may allow third world countries access to an effective and inexpensive antimalarial therapy to counter the estimated half billion infections that occur annually.

IT 865788-35-8P

RN

RN

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(oral farnesyltransferase inhibitors preparation as antimalarial drugs) 865788-35-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-[(2-methylphenyl)methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \end{array} \right) \begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{N} \end{array}$$

IT 865788-27-8P 865788-30-3P 865788-31-4P 865788-32-5P 865788-33-6P 865788-34-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(oral farnesyltransferase inhibitors preparation as antimalarial drugs) 865788-27-8 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl-N-(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2-\text{Ph} \\ \text{O} \\ \text{Me} \end{array}$$

RN 865788-30-3 HCAPLUS

CN Benzenesulfonamide, N-[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-31-4 HCAPLUS

CN 1-Naphthalenesulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-5-(dimethylamino)-N-(phenylmethyl)- (CA INDEX NAME)

RN 865788-32-5 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-[2-[(4-cyanophenyl)](1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-N-(cyclohexylmethyl)-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{CH}_2 - \text{N} - \text{CH}_2 - \text{CH}_2 - \text{N} \\ \end{array} \right) \begin{array}{c} \text{CH}_2 \\ \text{S} \\ \text{N} \end{array}$$

RN 865788-33-6 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl][(1-methyl-1H-imidazol-4-yl)sulfonyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{CH}_2 - \text{C}_{-\text{NHBu-t}} \\ \text{N} \\ \text{N} \\ \text{CH}_2 - \text{N}_{-\text{CH}_2} - \text{CH}_2 - \text{N}_{-\text{S}} \\ \text{Me} \end{array}$$

RN 865788-34-7 HCAPLUS

CN 1H-Imidazole-4-sulfonamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-[(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-1-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \end{array} \right) \xrightarrow{\text{Me}} \\ \text{Me} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{N} \\ \text$$

IT 865788-39-2P 865788-42-7P 865788-43-8P 865788-44-9P 865788-45-0P 865788-46-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(oral farnesyltransferase inhibitors preparation as antimalarial drugs)

RN 865788-39-2 HCAPLUS

CN Carbamic acid, [2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c}
\text{CH}_2 - \text{CH}_2 - \text{NH} - \text{C} - \text{OBu-t} \\
\text{N} - \text{CH}_2 - \text{N} - \text{C} - \text{OBu-t}
\end{array}$$

RN 865788-42-7 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[(phenylmethyl)amino]ethyl]amino]- (CA INDEX NAME)

RN 865788-43-8 HCAPLUS

CN Benzonitrile, 4-[[2-[(cyclohexylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

RN 865788-44-9 HCAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)]((1-methyl-1H-imidazol-5-yl)methyl]amino]ethyl]amino]-N-(1,1-dimethylethyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{NHBu-t} \\ \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{CH}_2 - \text{CH}_2 - \text{C} \\ \text{C} \\ \text{C} - \text{C} \\ \text{C} - \text{C} \\ \text{C} - \text{C} \\$$

RN 865788-45-0 HCAPLUS

CN Benzonitrile, 4-[[2-[([1,1'-biphenyl]-4-ylmethyl)amino]ethyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

$$\begin{array}{c}
\text{Ph} \\
\text{CN}
\end{array}$$

RN 865788-46-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl][2-[[(2-methylphenyl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N}
\end{array}$$

$$\begin{array}{c}
\text{Me} \\
\text{CH}_2 - \text{NH} - \text{CH}_2 - \text{NH} - \text{CH}_2
\end{array}$$

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 11 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:402307 HCAPLUS Full-text

DOCUMENT NUMBER: 140:406807

TITLE: Preparation of 1-phenylamino-1H-imidazoles as

aromatase inhibitors

INVENTOR(S): Adje, Nathalie; Bonnet, Paule; Carniato, Denis;

Delansorne, Remi; Lafay, Jean; Pascal, Jean-Claude

PATENT ASSIGNEE(S): Laboratoire Theramex, Monaco

SOURCE: U.S., 13 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND DATE			APPLICATION NO.						DATE				
US 6737433				B1 20040518				US 2002-319840						20021216				
EP	EP 1431292				A1 20040623					EP 2002-293107					20021216			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	SK			
CA	2510	175			A1		2004	0701	1	CA 2	003-	2510	175		2	0031	215	
WO	WO 2004054983 A2				A2		2004	0701	WO 2003-EP15027						20031215			
WO	2004	0549	83		А3		2004	0805										
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AΖ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
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		GE,	GH,	GM,	HR,	HU,	ID,	IL.	IN.	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	

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            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
            ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
            TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                        A1
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                                         HK 2006-103250
                                                                 20060314
                                                             A 20021216
PRIORITY APPLN. INFO.:
                                          EP 2002-293107
                                                              A 20021216
                                          US 2002-319840
                                          WO 2003-EP15027 W 20031215
OTHER SOURCE(S):
                        CASREACT 140:406807; MARPAT 140:406807
ED
    Entered STN: 18 May 2004
GΙ
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AΒ

= 0-2; R3, R4, R5, R6 = independently H, alkyl, cyano, alkoxy, CF3, alkylthio, alkylsulfonyl, sulfonamido, acyl, alkoxycarbonyl, carboxamido; R3CCR6 = benzofuran, N-methylbenzotriazole; their acid addition salts, solvates and stereoisomeric forms] were prepared as aromatase inhibitors, in particular for controlling and managing reproduction functions, and treatment of related tumors. For example, II was prepared, in 60%, by N-arylation of N-(1H-Imidazol-1-yl)-4-trifluoromethylaniline with 4-fluorobenzonitrile in DMSO. III•HCl displayed an IC50 = $0.18 \cdot -+$. 0.02 nM for the inhibition of human aromatase in vitro. III•HCl showed 57-59% inhibition of aromatase in vivo. Selected I are inhibitors of estrogen biosynthesis in vivo. ΙT 690248-14-7P, 4-[N-(1H-Imidazol-1-yl)-N-(4trifluoromethylphenylmethyl)amino]benzonitrile 690248-24-9P, 4-[N-(1H-Imidazol-1-yl)-N-(4-chlorophenylmethyl)amino]benzonitrile hydrochloride 690248-25-0P, 4-[N-(1H-Imidazol-1-yl)-N-(4-yl)]methoxyphenylmethyl)amino]benzonitrile hydrochloride 690248-26-1P , 4-[N-(1H-Imidazol-1-vl)-N-[(3-fluoro-4-methoxyphenvl)methyl]amino]benzonitrile hydrochloride 690248-27-2P, 4-[N-(1H-Imidazol-1-yl)-N-(4-yl)]methylphenylmethyl)amino]benzonitrile 690248-28-3P, 4-[N-(1H-Imidazol-1-yl)-N-(4-cyanophenylmethyl)amino]benzonitrile hydrochloride 690248 - 29 - 4P, 4 - [N - (1H - Imidazol - 1 - yl) - N - [(3, 4 - yl)] - N - [(3, 4 - ydimethoxyphenyl)methyl]amino]benzonitrile hydrochloride 690248-31-8P 690248-32-9P, 4-[N-(1H-Imidazol-1-yl)-N-[(4methylthiophenyl)methyl]amino]benzonitrile 690248-33-0P,

Title compds. I [wherein R1, R2 = independently H, cyclo/alkyl; X = (CH2)n; n

```
4-[N-(1H-Imidazol-1-yl)-N-[(4-methylsulfonylphenyl)methyl]amino]benzonitri
le 690248-34-1P, 4-[N-(1H-Imidazol-1-yl)-N-(3,4-1P)]
difluorophenylmethyl)amino]benzonitrile 690248-35-2P,
4-[N-(1H-Imidazol-1-yl)-N-(2,4-difluorophenylmethyl)amino]benzonitrile
690248-36-3P, 4-[N-(1H-Imidazol-1-yl)-N-(3,5-
difluorophenylmethyl)amino]benzonitrile 690248-37-4P,
4-[N-(1H-Imidazol-1-yl)-N-(4-bromophenylmethyl)amino]benzonitrile
hydrochloride 690248-41-0P, 4-[N-(1H-Imidazol-1-yl)-N-
(phenylmethyl)amino]benzonitrile 690248-43-2P,
4-[N-(1H-Imidazol-1-yl)-N-(3-fluorophenylmethyl) amino] benzonitrile
690248-44-3P, Methyl 4-[N-(4-cyanophenyl)-N-(1H-imidazol-1-
yl)amino]methyl]benzoate 690248-46-5P, 4-[N-(1H-Imidazol-1-yl)-N-
(3-trifluoromethylphenylmethyl)amino]benzonitrile 690248-50-1P,
4-[N-(4-Methyl-1H-imidazol-1-yl)-N-(4-bromophenylmethyl) amino] benzonitrile
690248-51-2P, 4-[N-(5-Methyl-1H-imidazol-1-yl)-N-(4-Methyl-1H-imidazol-1-yl)]
bromophenylmethyl)amino]benzonitrile 690248-52-3P,
4-[N-(4,5-Dimethyl-1H-imidazol-1-yl)-N-(4-bromophenylmethyl) amino] benzonit
rile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (aromatase inhibitor; preparation of 1-phenylamino-1H-imidazoles as
   aromatase inhibitors)
690248-14-7 HCAPLUS
Benzonitrile, 4-[1H-imidazol-1-yl[[4-(trifluoromethyl)phenyl]methyl]amino]-
  (CA INDEX NAME)
```

RN

CN

● HCl

● HCl

RN 690248-26-1 HCAPLUS
CN Benzonitrile, 4-[[(3-fluoro-4-methoxyphenyl)methyl]-1H-imidazol-1-ylamino], hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ CH2 \\ \end{array}$$
 CN
$$\begin{array}{c} CN \\ CH2 \\ \end{array}$$
 OMe

● HCl

RN 690248-27-2 HCAPLUS
CN Benzonitrile, 4-[1H-imidazol-1-yl[(4-methylphenyl)methyl]amino]- (CA INDEX NAME)

● HCl

RN 690248-29-4 HCAPLUS

CN Benzonitrile, 4-[[(3,4-dimethoxyphenyl)methyl]-1H-imidazol-1-ylamino]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 690248-31-8 HCAPLUS

CN Benzonitrile, 4-[[(4-fluorophenyl)methyl]-1H-imidazol-1-ylamino]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 690248-32-9 HCAPLUS

CN Benzonitrile, 4-[1H-imidazol-1-yl[[4-(methylthio)phenyl]methyl]amino]-(CA INDEX NAME)

RN 690248-33-0 HCAPLUS
CN Benzonitrile, 4-[1H-imidazol-1-yl[[4-(methylsulfonyl)phenyl]methyl]amino](CA INDEX NAME)

RN 690248-34-1 HCAPLUS
CN Benzonitrile, 4-[[(3,4-difluorophenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 690248-35-2 HCAPLUS
CN Benzonitrile, 4-[[(2,4-difluorophenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 690248-36-3 HCAPLUS
CN Benzonitrile, 4-[[(3,5-difluorophenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

● HCl

RN 690248-41-0 HCAPLUS CN Benzonitrile, 4-[1H-imidazol-1-yl(phenylmethyl)amino]- (CA INDEX NAME)

RN 690248-43-2 HCAPLUS
CN Benzonitrile, 4-[[(3-fluorophenyl)methyl]-1H-imidazol-1-ylamino]- (CA INDEX NAME)

RN 690248-44-3 HCAPLUS
CN Benzoic acid, 4-[[(4-cyanophenyl)-1H-imidazol-1-ylamino]methyl]-, methyl ester (CA INDEX NAME)

RN 690248-46-5 HCAPLUS
CN Benzonitrile, 4-[1H-imidazol-1-yl[[3-(trifluoromethyl)phenyl]methyl]amino](CA INDEX NAME)

RN 690248-50-1 HCAPLUS
CN Benzonitrile, 4-[[(4-bromophenyl)methyl](4-methyl-1H-imidazol-1-yl)amino](CA INDEX NAME)

RN 690248-51-2 HCAPLUS
CN Benzonitrile, 4-[[(4-bromophenyl)methyl](5-methyl-1H-imidazol-1-yl)amino](CA INDEX NAME)

RN 690248-52-3 HCAPLUS
CN Benzonitrile, 4-[[(4-bromophenyl)methyl](4,5-dimethyl-1H-imidazol-1-yl)amino]- (CA INDEX NAME)

IT 690248-15-8P, 4-[N-(2,3-Dihydro-1H-imidazol-1-yl-2-thione)-N-(4-midazol-1-yl-2-thione)]

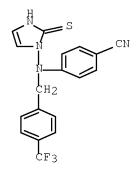
trifluoromethylphenylmethyl)amino]benzonitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 1-phenylamino-1H-imidazoles as aromatase inhibitors)

RN 690248-15-8 HCAPLUS

CN Benzonitrile, 4-[(2,3-dihydro-2-thioxo-1H-imidazol-1-yl)][[4-(trifluoromethyl)phenyl]methyl]amino]- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 12 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:570981 HCAPLUS Full-text

DOCUMENT NUMBER: 139:133571

TITLE: Preparation of heterocyclic compounds such as oxazoles

as anticancer agents

INVENTOR(S): Tasaka, Akihiro; Taniguchi, Takahiko; Takakura,

Nobuyuki; Momose, Yu; Naito, Kenichiro; Tsujimoto,

Saori

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 274 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

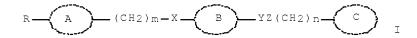
PATENT NO. KIND DATE APPLICATION NO. DATE

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                                           ______
    WO 2003059907
                         Α1
                               20030724
                                           WO 2003-JP310
                                                                  20030116
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            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
            LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
            PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
            UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    AU 2003203170
                               20030730
                                           AU 2003-203170
                         Α1
                                                                  20030116
    JP 2003277379
                               20031002
                                           JP 2003-8814
                                                                  20030116
                         Α
PRIORITY APPLN. INFO.:
                                           JP 2002-9255
                                                             A 20020117
                                           WO 2003-JP310
                                                             W 20030116
```

OTHER SOURCE(S): MARPAT 139:133571

ED Entered STN: 25 Jul 2003

GΙ



AB The title compds. I [A is a nitrogenous heterocycle; B is an optionally substituted aromatic homocycle or an optionally substituted aromatic heterocycle; C is a 5- or 6-membered nitrogenous heterocycle which may be substituted; R is an optionally substituted aromatic homocyclic group or the like; m is an integer of 0 to 2; n is an integer of 1 to 5; X is oxygen or the like; and Y and Z may be the same or different from each other and are each a single bond, an oxygen atom, an optionally substituted carbon atom, or the like] are prepared Compds. of this invention in vitro showed IC50 values of < 0.05 $\mu \rm M$ to 0.2 $\mu \rm M$ against the growth of breast cancer cells BT-474. Formulations containing I are given.

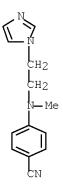
IT 568594-05-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic compds. such as oxazole derivs. as anticancer agents)

RN 568594-05-8 HCAPLUS

CN Benzonitrile, 4-[[2-(1H-imidazol-1-yl)ethyl]methylamino]- (CA INDEX NAME)



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 13 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:236032 HCAPLUS Full-text

DOCUMENT NUMBER: 139:133506

TITLE: Novel and selective imidazole-containing biphenyl

inhibitors of protein farnesyltransferase

AUTHOR(S): Curtin, Michael L.; Florjancic, Alan S.; Cohen,

Jerome; Gu, Wen-Zhen; Frost, David J.; Muchmore,

Steven W.; Sham, Hing L.

CORPORATE SOURCE: Global Pharmaceutical Research and Development,

Departments of Cancer Research and Advanced

Technology, Abbott Laboratories, Abbott Park, IL,

60064, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003),

13(7), 1367-1371

CODEN: BMCLE8; ISSN: 0960-894X

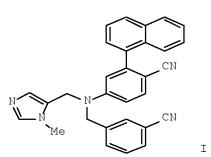
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:133506

ED Entered STN: 27 Mar 2003

GΙ



AB A series of imidazole-containing biphenyls was prepared and evaluated in vitro for inhibition of FTase and cellular Ras processing. Several of these analogs, e.g., I, are potent inhibitors of FTase (<1 nM), FTase/GGTase selective (>300-fold) and cellularly active (≤80 nM). An X-ray crystal structure of inhibitor I bound to rat farnesyltransferase is also presented.

IT 565451-86-7

RL: PAC (Pharmacological activity); BIOL (Biological study)
(farnesyltransferase inhibition and structure-activity relationships of biarylbenzylamines)

RN 565451-86-7 HCAPLUS

CN Benzonitrile, 4-[(1H-imidazol-5-ylmethyl)(phenylmethyl)amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

IT 565451-83-4P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, farnesyltransferase inhibition, SAR, and pharmacokinetics of N-(methylimidazolylmethyl)-N-(naphthylcyanophenyl)-benzylamine and crystal structure of complex with farnesyltransferase and hydroxyfarnesylphosphonic acid)

RN 565451-83-4 HCAPLUS

CN Benzonitrile, 4-[[(3-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{N} \\ \text{N} \\ \text{CH}_2 \\ \text{CN} \\ \end{array}$$

IT 371764-01-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, farnesyltransferase inhibition, and SAR of imidazolylbiarylamine via reductive condensation of tritylimidazolecarboxaldehyde with biarylamine followed by alkylation and deprotection)

RN 371764-01-1 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[(1H-imidazol-5-ylmethyl)(phenylmethyl)amino]-2'-methyl- (CA INDEX NAME)

IT 371766-31-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, farnesyltransferase inhibition, and SAR of imidazolylbiarylamine via reductive condensation of

tritylimidazolecarboxaldehyde with biarylamine followed by alkylation and deprotection)

RN 371766-31-3 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 2'-methyl-5-[(phenylmethyl)[[1-(triphenylmethyl)-1H-imidazol-4-yl]methyl]amino]- (CA INDEX NAME)

IT 371763-58-5P 371763-59-6P 371763-61-0P 371763-63-2P 371763-64-3P 371763-65-4P 371763-67-6P 371763-69-8P 565451-84-5P 565451-85-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, farnesyltransferase inhibition, and SAR of imidazolylbiarylamines via Suzuki coupling of chlorobenzoate with arylboronic acids followed by hydrolysis, amination, reductive condensation with imidazolecarboxaldehyde, and alkylation)

RN 371763-58-5 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 2'-methyl-5-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]- (CA INDEX NAME)

RN 371763-59-6 HCAPLUS

CN Benzonitrile, 4-[methyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N-CH}_2 \end{array}$$

RN 371763-61-0 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

$$\stackrel{\text{Me}}{\underset{\text{N}}{\bigvee}} \text{CH}_2 - \stackrel{\text{CN}}{\underset{\text{CH}_2}{\bigvee}} \text{Me}$$

RN 371763-63-2 HCAPLUS

CN Benzonitrile, 4-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{N} \\ \text{NC} \\ \text{CH}_2 \\ \text{N} \\ \text{CN} \\ \end{array}$$

RN 371763-64-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

RN 371763-65-4 HCAPLUS

CN Benzonitrile, 4-[hexyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

Me Me (CH₂) 5
$$CH_2 - N$$

$$CN$$

RN 371763-67-6 HCAPLUS

CN Benzamide, N-[4-cyano-3-(1-naphthalenyl)phenyl]-N-[(1-methyl-1H-imidazol-5-yl)methyl]- (CA INDEX NAME)

RN 371763-69-8 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(3-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

RN 565451-84-5 HCAPLUS

CN Benzonitrile, 4-[[(3-chlorophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ N \\ CH_2 \\ N \\ CH_2 \\ C1 \\ \end{array}$$

RN 565451-85-6 HCAPLUS

CN 2-Pyridinecarbonitrile, 4-[[[4-cyano-3-(1-naphthalenyl)phenyl]][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{N} \\ \text{NC} \\ \text{CH}_2 \\ \text{C} \\ \text{NC} \\ \text{C} \\ \text{NC} \\ \text{C} \\ \text{N} \\ \text{C} \\ \text{C} \\ \text{N} \\ \text{C} \\ \text{C$$

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 14 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2002:123617 HCAPLUS Full-text

DOCUMENT NUMBER: 136:183819

TITLE: Preparation of (imidazolylalkyl)biphenylcarbonitriles

and analogs as farnesyltransferase inhibitors

INVENTOR(S): Wang, Wei-Bo; Curtin, Michael L.; Fakhoury, Stephen

A.; Gwaltney, Stephen L.; Hasvold, Lisa A.; Hutchins, Charles W.; Li, Qun; Lin, Nan-Horng; Nelson, Lissa Taka Jennings; O'Connor, Steve; Sham, Hing L.;

Sullivan, Gerard M.; Wang, Gary T.; Wang, Xilu

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 189 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020019527	A1	20020214	US 2001-842391	20010425
PRIORITY APPLN. INFO.:			US 2000-200165P P	20000427
OTHER SOURCE(S):	MARPAT	136:183819		

ED Entered STN: 15 Feb 2002

GΙ

- AB Title compds. (I) were prepared Thus, 2-MeC6H4C6H3(CN)(CHO)-2,5 was condensed with 1-methyl-2-triethylsilyl-1H-imidazole (preparation each given) and the product O-arylated to give title compound II. Data for biol. activity of I were given.
- IT 371763-58-5P 371763-59-6P 371763-60-9P 371763-61-0P 371763-62-1P 371763-63-2P 371763-64-3P 371763-65-4P 371763-67-6P 371763-68-7P 371763-69-8P 371763-99-4P 371764-00-0P 371764-01-1P 371764-02-2P
 - RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 - (preparation of (imidazolylalkyl)biphenylcarbonitriles and analogs as farnesyltransferase inhibitors)
- RN 371763-58-5 HCAPLUS
- CN [1,1'-Biphenyl]-2-carbonitrile, 2'-methyl-5-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]- (CA INDEX NAME)

- RN 371763-59-6 HCAPLUS
- CN Benzonitrile, 4-[methyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

RN 371763-60-9 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl]-2-propen-1-ylamino]-2- (1-naphthalenyl)- (CA INDEX NAME)

RN 371763-61-0 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

$$\begin{array}{c} \stackrel{\text{Me}}{\underset{\text{N}}{\bigvee}} \text{CH}_2 - \stackrel{\text{CN}}{\underset{\text{CH}_2}{\bigvee}} \\ \stackrel{\text{CH}_2}{\underset{\text{CN}}{\bigvee}} \\ \end{array}$$

RN 371763-62-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl](3-phenylpropyl)amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

RN 371763-63-2 HCAPLUS

CN Benzonitrile, 4-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c} \text{N} \\ \text{NC} \\ \text{CH}_2 \\ \text{CN} \\ \end{array}$$

RN 371763-64-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]-2- (1-naphthalenyl)- (CA INDEX NAME)

RN 371763-65-4 HCAPLUS

CN Benzonitrile, 4-[hexyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

Me Me (CH₂) 5
$$CH_2 - N$$

$$CN$$

RN 371763-67-6 HCAPLUS

CN Benzamide, N-[4-cyano-3-(1-naphthalenyl)phenyl]-N-[(1-methyl-1H-imidazol-5-yl)methyl]- (CA INDEX NAME)

RN 371763-68-7 HCAPLUS

CN Benzamide, N-(6-cyano-2'-methyl[1,1'-biphenyl]-3-yl)-N-[(1-methyl-1H-imidazol-5-yl)methyl]- (CA INDEX NAME)

RN 371763-69-8 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(3-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

RN 371763-99-4 HCAPLUS

CN Benzoic acid, 4-[[[4-cyano-3-(1-naphthalenyl)phenyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]-, methyl ester (CA INDEX NAME)

RN 371764-00-0 HCAPLUS

CN Benzoic acid, 4-[[[4-cyano-3-(1-naphthalenyl)phenyl]][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]- (CA INDEX NAME)

$$_{\text{CH}_2}^{\text{N}}$$
 Me $_{\text{CH}_2}$

RN 371764-01-1 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[(1H-imidazol-5-ylmethyl)(phenylmethyl)amino]-2'-methyl- (CA INDEX NAME)

RN 371764-02-2 HCAPLUS

CN Benzoic acid, 3-[[[4-cyano-3-(1-naphthalenyl)phenyl]][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-C} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{CN} \\ \text{$$

L44 ANSWER 15 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2001:798200 HCAPLUS Full-text

TITLE: Preparation of substituted 4-

(heteroarylmethyl)benzonitriles as farnesyltransferase

inhibitors

INVENTOR(S): Wang, Wei-Bo; Curtin, Michael L.; Fakhoury, Stephen

A.; Gwaltney, Stephen L., II; Hasvold, Lisa A.; Hutchins, Charles W.; Li, Qui; Lin, Nan-Horng; Jennings Nelson, Lissa Taka; O'Connor, Stephen J.; Sham, Hing L.; Sullivan, Gerald M.; Wang, Gary T.;

Wang, Xilu

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 305 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	PATENT NO.			KIN	IND DATE			APPLICATION NO.						DATE			
	2001 2001								,	WO 2	001-	JS13	678		2	0010	425
	W:	AE, CR, HU, LU,	AG, CU, ID, LV, SE,	AL, CZ, IL, MA,	AM, DE, IN, MD,	AT, DK, IS, MG,	AU, DM, JP, MK,	AZ, DZ, KE, MN, TJ,	EE, KG, MW,	ES, KP, MX,	FI, KR, MZ,	GB, KZ, NO,	GD, LC, NZ,	GE, LK, PL,	GH, LR, PT,	GM, LS, RO,	HR, LT, RU,
CA	RW:	GH, DE, BJ,	GM, DK,	ES,	FI, CI,	FR, CM,	GB, GA,	SD, GR, GN,	IE, GW,	IT, ML,	LU, MR,	MC, NE,	NL, SN,	PT, TD,	SE, TG	TR,	BF,
EP	1276 R:	AT,		,	DE,	DK,	ES,	0122 FR, MK,	GB,	GR,	IT,						
	2004 2002 Y APP	PA10	608						1	JP 20 MX 20 US 20 US 20 WO 20	002- 000- 001-	PA10 5632 8222	608 56 05	1	2 A 2 A 2	0010 0021 0000 0010 0010	025 427 402
OFFIED 0		<i>(</i> \(\) \(\)			1 (T T)	m	100	0 4 4 4	^ ^								

OTHER SOURCE(S): MARPAT 135:344482

ED Entered STN: 02 Nov 2001

GI

$$\mathbb{R}^{2} \xrightarrow{\mathbb{A}^{1}} \mathbb{C}^{\mathbb{N}}$$

AB The title compds. [I; A1 = (un)substituted alkylene, etc.; R1 = halo, cycloalkyl, aryl, heteroaryl; R2 = heteroaryl selected from imidazolyl, pyrazolyl, pyrrolyl, etc.] and their pharmaceutically acceptable salts which farnesyltransferase, were prepared E.g., 3-step synthesis of the benzonitrile II.HCl which 88% inhibition of farnesyltransferase at 10-6 M, was given.

IT 371763-99-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted 4-(heteroarylmethyl)benzonitriles as farnesyltransferase inhibitors)

RN 371763-99-4 HCAPLUS

CN Benzoic acid, 4-[[[4-cyano-3-(1-naphthalenyl)phenyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} \text{MeO-C} \\ \\ \text{CH}_2 \\ \\ \text{CN} \\ \end{array}$$

IT 371763-58-5P 371763-59-6P 371763-60-9P 371763-61-0P 371763-62-1P 371763-63-2P 371763-64-3P 371763-65-4P 371763-67-6P 371763-68-7P 371763-69-8P 371764-00-0P 371764-01-1P 371764-02-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted 4-(heteroarylmethyl)benzonitriles as farnesyltransferase inhibitors)

RN 371763-58-5 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 2'-methyl-5-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]- (CA INDEX NAME)

RN 371763-59-6 HCAPLUS

CN Benzonitrile, 4-[methyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

RN 371763-60-9 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl]-2-propen-1-ylamino]-2- (1-naphthalenyl)- (CA INDEX NAME)

RN 371763-61-0 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

$$\begin{array}{c} \stackrel{\text{Me}}{\underset{\text{N}}{\bigvee}} \text{CH}_2 - \stackrel{\text{CN}}{\underset{\text{CH}_2}{\bigvee}} \\ \stackrel{\text{CH}_2}{\underset{\text{CN}}{\bigvee}} \end{array}$$

RN 371763-62-1 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl](3-phenylpropyl)amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c}
\text{Me} \\
\text{N} \\
\text{CH}_2 - \text{N}
\end{array}$$

RN 371763-63-2 HCAPLUS

CN Benzonitrile, 4-[[(4-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & \\ & &$$

RN 371763-64-3 HCAPLUS

CN Benzonitrile, 4-[[(1-methyl-1H-imidazol-5-yl)methyl](phenylmethyl)amino]-2- (1-naphthalenyl)- (CA INDEX NAME)

RN 371763-65-4 HCAPLUS

CN Benzonitrile, 4-[hexyl[(1-methyl-1H-imidazol-5-yl)methyl]amino]-2-(1-naphthalenyl)- (CA INDEX NAME)

Me Me (CH₂) 5
$$CH_2 - N$$

$$CN$$

RN 371763-67-6 HCAPLUS

CN Benzamide, N-[4-cyano-3-(1-naphthalenyl)phenyl]-N-[(1-methyl-1H-imidazol-5-yl)methyl]- (CA INDEX NAME)

RN 371763-68-7 HCAPLUS

CN Benzamide, N-(6-cyano-2'-methyl[1,1'-biphenyl]-3-yl)-N-[(1-methyl-1H-imidazol-5-yl)methyl]- (CA INDEX NAME)

RN 371763-69-8 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[[(3-cyanophenyl)methyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]-2'-methyl- (CA INDEX NAME)

RN 371764-00-0 HCAPLUS

CN Benzoic acid, 4-[[[4-cyano-3-(1-naphthalenyl)phenyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]- (CA INDEX NAME)

$$_{\text{CH}_2}^{\text{N}}$$
 Me $_{\text{CH}_2}^{\text{N}}$ CN

RN 371764-01-1 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 5-[(1H-imidazol-5-ylmethyl)(phenylmethyl)amino]-2'-methyl- (CA INDEX NAME)

RN 371764-02-2 HCAPLUS

CN Benzoic acid, 3-[[[4-cyano-3-(1-naphthalenyl)phenyl][(1-methyl-1H-imidazol-5-yl)methyl]amino]methyl]-, methyl ester (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ CH_2 \\ \end{array}$$

IT 371766-31-3

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of substituted 4-(heteroarylmethyl)benzonitriles as farnesyltransferase inhibitors)

RN 371766-31-3 HCAPLUS

CN [1,1'-Biphenyl]-2-carbonitrile, 2'-methyl-5-[(phenylmethyl)[[1-(triphenylmethyl)-1H-imidazol-4-yl]methyl]amino]- (CA INDEX NAME)

L44 ANSWER 16 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1998:228992 HCAPLUS Full-text

DOCUMENT NUMBER: 128:257449

ORIGINAL REFERENCE NO.: 128:50967a,50970a

TITLE: Preparation and anti-HIV activity of substituted

diamino-1,3,5-triazine derivatives

INVENTOR(S): Kukla, Michael Joseph; Ludovici, Donald W.; Janssen,

Paul Adriaan Jan; Heeres, Jan; Moereels, Henri Emiel

Lodewijk

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND		DATE			APF	PLIC.	ATI	ON I	NO.		D	DATE		
EP	8345	07			A1		19980			EP	199	7-2	029	 17		1	9970	924
EP	8345				В1													
	R:						ES,	FR,	GB,	GF	R, I	Τ,	LI,	LU,	NL,	SE,	MC,	PT,
			SI,	LT,	LV,	FI,												
	9704				А		1998			ИО	199	7 - 4	1368			1	9970	922
	3116				В1		2001											
	2973				В6		2006				199						9970	
	2671				T		20040							17			9970	
	8345				T		2004				199						9970	
	2221				T3		2005				199						9970	
	2216				A1		1998				199						9970	
	1997		740		Α		2005				199						9970	
	9739				А		1998			AU	199	7–3	926	6		1	9970	926
	7408				В2		2001											
	3288				А		2000				199						9970	
	6380				В1		20020				199			02			9970	
	3826				В1		2002				199						9970	
	1011				A		1998			JP	199	7-2	:793	87		1	9970	929
	4127	882			В2		2008											
AP	914 w.	KE,	IIC	7.M	A ZM		20001	1218		AP	199	7-1	.109			1	9970	929
TT.	1218		00,	۵1.1	A		2001	1826		TT.	199	7_1	218	19		1	9970	929
	2852				В6		2006				199						9970	
	1180				A		19980				199						9970	
_	1083				C		20020			011	100	, -		<i>J</i> 1		_	3370	,,,,
	9708				A		1999			7.A	199	7-8	766			1	9970	930
	9701				A2		1999				199						9970	
	9701				A3		20000					_					33,0	
	2252				B1		2006											
	9704				A		20000			BR	199	7-4	937			1	9970	930
	4113				В		20003							4172			9970	
	2186						2002				199						9970	
	9705				B1		2002				199						9970	
	1901				B1		2005				199			69			9970	
	1009				A1		2004				199						9980	
	2002		181		A1		2002				200						0011	
	6858				В2		2005											
	2003		473		A1		2003			US	200	3-3	977	60		2	0030	326
	6962		-		В2		2005							-		_		-
	2006		614		A1		2006			US	200	5-2	033	25		2	0050	812
	APP			. :										0P			9961	
	_										199						9970	
											200	_				_	0011	
RIT	(APP	LN.	INFO	. :						US	199	7-9	386	02		A3 1	9970	9:

US 2003-397760 A3 20030326

OTHER SOURCE(S): MARPAT 128:257449

ED Entered STN: 23 Apr 1998

GΙ

The title compds. I [R1, R2 = hydrogen, hydroxy, amino, optionally substituted AΒ C1-6alkyl, C1-6alkyloxy, C1-6alkylcarbonyl, C1-6alkyloxycarbonyl, Arl, monoor di(C1-6alkyl)amino, mono- or di(C1-6alkyl)aminocarbonyl, dihydro-2(3H)furanone, or R1 and R2 taken together may form pyrrolidinyl, piperidinyl, morpholinyl, azido or mono- or di(C1-6alkyl)aminoC1-4alkylidene; R3 = hydrogen, Ar1, C1-6alkylcarbonyl, C1-6alkyl, C1-6alkyloxycarbonyl, C1-6alkyl substituted with C1-6alkyloxycarbonyl; R4, R5, R6, R7, R8 = hydrogen, halo, C1-6alkyl, C1-6alkyloxy, cyano, aminocarbonyl, nitro, amino, trihalomethyl, trihalomethyloxy; L = optionally substituted C1-10alkyl, C3-10alkenyl, C3-10alkynyl, C3-7cycloalkyl; Ar1 = optionally substituted phenyl], useful for the manufacture of a medicine for the treatment of subjects suffering from HIV (Human Immunodeficiency Virus) infection, were prepared E.g., reaction of Ph N'-cyano-N-(4-cyanophenyl)carbamimidate, prepared from 4-cyanoaniline and di-Ph N-cyanocarbonimidate, with 2,6-dichlorobenzeneethanimidamide gave 67% 4-[[4-amino-6-[(2,6-dichlorophenyl)methyl]-1,3,5-triazin-2vllaminolbenzonitrile.

IT 205381-44-8P 205381-45-9P 205381-46-0P 205381-48-2P 205381-49-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and anti-HIV activity of diaminotriazines)

RN 205381-44-8 HCAPLUS

CN Glycine, N-[4-amino-6-[(2,6-dichlorophenyl)methyl]-1,3,5-triazin-2-yl]-N- (4-cyanophenyl)-, methyl ester (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & &$$

RN 205381-45-9 HCAPLUS

CN Acetamide, N-[4-(acetylamino)-6-[(2,6-dichlorophenyl)methyl]-1,3,5-triazin-2-yl]-N-(4-cyanophenyl)- (CA INDEX NAME)

RN 205381-46-0 HCAPLUS

CN Imidodicarbonic acid, N-[4-[(4-cyanophenyl)(ethoxycarbonyl)amino]-6-[(2,6-dichlorophenyl)methyl]-1,3,5-triazin-2-yl]-, C,C'-diethyl ester (CA INDEX NAME)

RN 205381-48-2 HCAPLUS

CN Acetamide, N-acetyl-N-[4-[acetyl(4-cyanophenyl)amino]-6-[(2,6-dichlorophenyl)methyl]-1,3,5-triazin-2-yl]- (CA INDEX NAME)

RN 205381-49-3 HCAPLUS

CN Carbamic acid, (4-cyanophenyl)[4-[(2,6-dichlorophenyl)methyl]-6[(ethoxycarbonyl)amino]-1,3,5-triazin-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 17 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN 1998:562758 HCAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 129:244681

ORIGINAL REFERENCE NO.: 129:49817a,49820a

A facile synthesis of trifluoromethylamines by TITLE:

oxidative desulfurization-fluorination of

dithiocarbamates

Kanie, Kiyoshi; Mizuno, Katsuya; Kuroboshi, Manabu; AUTHOR(S):

Hiyama, Tamejiro

CORPORATE SOURCE: Research Laboratory of Resources Utilization, Tokyo

Institute of Technology, Midori-ku, Yokohama,

Kanagawa, 226-8503, Japan

SOURCE: Bulletin of the Chemical Society of Japan (1998),

71(8), 1973-1991

CODEN: BCSJA8; ISSN: 0009-2673

Chemical Society of Japan PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:244681

Entered STN: 04 Sep 1998

Trifluoromethylamines are easily synthesized from dithiocarbamates by a AΒ reagent system consisting of tetrabutylammonium dihydrogen trifluoride and an N-halo imide under mild conditions. When this reaction was applied to dithiocarbamates ArN(R)CS2Me at higher temps., the trifluoromethylation was accompanied by halogen substitution at the p-position of the Ar group. The synthesis of trifluoromethyl-substituted adenosine is also described.

143490-24-8P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of trifluoromethylamines by oxidative desulfurizationfluorination of dithiocarbamates)

RN 143490-24-8 HCAPLUS

Benzonitrile, 4-[(phenylmethyl)(trifluoromethyl)amino]- (CA INDEX NAME) CN

THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 33 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 18 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1997:213310 HCAPLUS Full-text

DOCUMENT NUMBER: 126:293338

ORIGINAL REFERENCE NO.: 126:56805a,56808a

TITLE: Studies on aromatase inhibitors. III. Synthesis and

> biological evaluation of [(4-bromobenzyl)(4cyanophenyl) amino] azoles and their azine analogs

Okada, Minoru; Yoden, Toru; Kawaminami, Eiji; Shimada, AUTHOR(S):

Yoshiaki; Kudoh, Masafumi; Isomura, Yasuo

CORPORATE SOURCE: Medicinal Chemistry Research II, Institute for Drug

Discovery Research, Yamanouchi Pharmaceutical Co.,

Ltd., Tsukuba, 305, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1997), 45(3),

482-486

CODEN: CPBTAL; ISSN: 0009-2363 Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:293338

ED Entered STN: 02 Apr 1997

GΙ

PUBLISHER:

AB A series of [(4-bromobenzyl)(4-cyanophenyl)amino]azoles and their azine analogs I (Ar = 3-pyridazinyl, 1,3,4-thiadiazol-2-yl, 3-pyridyl, etc.), which have the side chain of the selective aromatase inhibitor YM511, were synthesized and evaluated for aromatase-inhibitory activity (in vitro) and for pregnant mare serum gonadotropin (PMSG)-induced estrogen synthesis inhibitory activity (in vivo). Among these aza-heterocycles, the pyrimidin-5-yl derivative I (R = pyrimidin-5-yl) (II) was the most potent aromatase inhibitor and its in vitro inhibitory activity was comparable to that of YM511. II also showed weak inhibitory activity on aldosterone synthesis. These data indicated that the pyrimidin-5-yl moiety is useful as a new azole fragment in place of the 4H-1,2,4-triazol-4-yl moiety of the aromatase inhibitor YM511.

IT 157911-83-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, aromatase inhibition, and estrogen and aldosterone synthesis inhibitory activity of (bromobenzyl)(cyanophenyl)amino-azoles and -azines)

RN 157911-83-6 HCAPLUS

CN Benzonitrile, 4-[[(4-bromophenyl)methyl]-1,2,4-triazin-3-ylamino]- (CA INDEX NAME)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 19 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1994:605372 HCAPLUS $\underline{\text{Full-text}}$

DOCUMENT NUMBER: 121:205372

ORIGINAL REFERENCE NO.: 121:37397a,37400a

TITLE: Preparation of aminopyrimidines as aromatase

inhibitors

INVENTOR(S): Okada, Minoru; Yoden, Toru; Kawaminami, Eiji; Shimada,

Yoshiaki; Kudo, Masafumi; Isomura, Yasuo

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	TENT :	NO.			KIN:	D	DATE			APP]	LICAT	ION :	NO.		D	ATE	
WO	9322	 290			A1	_	1993	1111		 WO :	 1993-	 JP54	8		1	 9930	427
	W:	ΑU,	BB,	BG,	BR,	CA,	CZ,	FΙ,	HU,	JP,	, KR,	KΖ,	LK,	MG,	MN,	MW,	NO,
		NΖ,	PL,	PT,	RO,	RU,	SD,	SK,	UA,	US,	, VN						
	RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	, IE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML	, MR,	ΝE,	SN,	TD,	ΤG		
AU	9340	230			Α		1993	1129		AU :	1993-	4023	0		1	9930	427
EP	6405	95			A1		1995	0301		EP :	1993-	9094	28		1	9930	427
EP	6405	95			В1		1999	0324									
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	, IE,	ΙT,	LI,	LU,	NL,	PT,	SE
AT	1780	56			Τ		1999	0415		AT :	1993-	9094	28		1	9930	427
ES	2130	258			Т3		1999	0701		ES :	1993-	9094	28		1	9930	427
CN	1079	962			Α		1993	1229		CN :	1993-	1053	30		1	9930	428
CN	1039	228			С		1998	0722									
US	5538	976			Α		1996	0723		US :	1994-	3253	83		1	9941	026
PRIORIT	Y APP	LN.	INFO	.:						JP :	1992-	1377	62		A 1	9920	428
										JP :	1992-	2342	98		A 1	9920	810
										WO :	1993-	JP54	8		A 1	9930	427

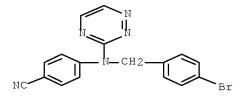
OTHER SOURCE(S): CASREACT 121:205372; MARPAT 121:205372

- ED Entered STN: 29 Oct 1994
- GI For diagram(s), see printed CA Issue.
- AB The title compds. I [A = single bond, alkylene, etc.; ring B = pyrimidine, pyridazine, triazine ring; rings D and E = (substituted) aryl, etc.; a proviso is given] were prepared I have aromatase inhibiting activity and are useful as therapeutic agents for breast cancer, endometriosis, prostatic hypertrophy, etc. Treatment of aminopyrimidine II with NaH in DMF, followed by reaction with 4-trifluoromethylbenzyl bromide, gave, after workup, title compound III. One compound I in vitro exhibited IC50 of 0.036 nM against aromatase. Formulations containing I are given.
- IT 157911-83-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as aromatase inhibitor)

- RN 157911-83-6 HCAPLUS
- CN Benzonitrile, 4-[[(4-bromophenyl)methyl]-1,2,4-triazin-3-ylamino]- (CA INDEX NAME)



L44 ANSWER 20 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1993:495073 HCAPLUS Full-text

DOCUMENT NUMBER: 119:95073

ORIGINAL REFERENCE NO.: 119:17133a,17136a

TITLE: Preparation of anticancer aromatic

N-triluoromethylamines

INVENTOR(S): Hyama, Tamejiro; Kuroboshi, Manabu; Wakakuri, Shinobu

PATENT ASSIGNEE(S): Sagami Chem Res, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
JP 05078286	А	19930330	JP 1991-268280	19910919		
JP 3083186	B2	20000904				
PRIORITY APPLN. INFO.:			JP 1991-268280	19910919		

OTHER SOURCE(S): CASREACT 119:95073; MARPAT 119:95073

ED Entered STN: 04 Sep 1993

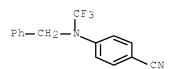
AB R1NR2CF3 [R1 = (un)substituted aryl; R2 = (un)substituted linear or branched alkyl; NR1R2 may form ring] are safely and easily prepared by treatment of R1NR2CS2R3 [R1, R2 = same as above; R3 = (un)substituted aryl, (un)substituted linear or branched alkyl] with F+ sources in the presence of halonium generators. Treatment of Me N-benzyl-N-(4- methoxyphenyl)dithiocarbamate with (Bu4N+)(H2F3-) and NBS in CH2Cl2 at room temperature for 1 h gave 97% N-benzyl-N-(4-methoxyphenyl)-N- trifloromethylamine, which inhibited murine leukemia P388 cell with IC50 of 4.9 μ g/mL.

IT 143490-24-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, by fluorination of dithiocarbamate derivative)

RN 143490-24-8 HCAPLUS

CN Benzonitrile, 4-[(phenylmethyl)(trifluoromethyl)amino]- (CA INDEX NAME)



DOCUMENT NUMBER: 117:150619

ORIGINAL REFERENCE NO.: 117:26085a,26088a

TITLE: A facile synthesis of trifluoromethylamines by

oxidative desulfurization-fluorination of

dithiocarbamates

AUTHOR(S): Kuroboshi, Manabu; Hiyama, Tamejiro

CORPORATE SOURCE: Sagami Chem. Res. Cent., Sagamihara, 229, Japan

SOURCE: Tetrahedron Letters (1992), 33(29), 4177-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:150619

ED Entered STN: 17 Oct 1992

AB Reaction of Me dithiocarbamates R1R2NC(S)SMe (e.g., R1 = 4-MeOC6H4, R2 = PhCH2) with Bu4N+ H2F3- and N-bromosuccinimide provides trifluoromethylamines

R1R2NCF3 in 62-99% yields.

IT 143490-24-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 143490-24-8 HCAPLUS

CN Benzonitrile, 4-[(phenylmethyl)(trifluoromethyl)amino]- (CA INDEX NAME)

L44 ANSWER 22 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1990:206483 HCAPLUS Full-text

DOCUMENT NUMBER: 112:206483

ORIGINAL REFERENCE NO.: 112:34743a,34746a

TITLE: Electrolytic transformation of fluoroorganic

compounds. 5. Anodic cyanation of

2,2,2-trifluoroethylamines

AUTHOR(S): Konno, Akinori; Fuchigami, Toshio; Fujita, Yasushi;

Nonaka, Tsutomu

CORPORATE SOURCE: Tokyo Inst. Technol., Grad. Sch. Nagatsuta, Yokohama,

227, Japan

SOURCE: Journal of Organic Chemistry (1990), 55(6), 1952-4

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English ED Entered STN: 26 May 1990

AB Regioselectivity of the anodic cyanation reaction of various types of 2,2,2-trifluoroethylamines was investigated. A remarkable difference in the

regioselectivity between the anodic cyanation and methoxylation of the trifluoroethylamines was observed. The cyano group was introduced into the $\alpha-$ position to the nitrogen atom other than the trifluoroethyl group. The effect of the trifluoromethyl group on the anodic substitution reactions and the

reaction mechanism are discussed. The acidity of the cation radicals of the amines and the basicity of the reaction medium were proposed as main factors for controlling regionelectivity in the anodic cyanation.

IT 126422-69-3P 126422-72-8P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in anodic cyanation of trifluoroethylamines, regioselectivity in relation to)

RN 126422-69-3 HCAPLUS

CN Benzonitrile, 4-[methyl(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

126422-72-8 HCAPLUS RN

CN Benzonitrile, 4-[ethyl(2,2,2-trifluoroethyl)amino]- (CA INDEX NAME)

L44 ANSWER 23 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:191866 HCAPLUS Full-text

DOCUMENT NUMBER: 100:191866 ORIGINAL REFERENCE NO.: 100:29175a

TITLE: Fungicidal heterocyclic amines

INVENTOR(S): Krumkalns, Eriks Victor; Smiley, David Lee

PATENT ASSIGNEE(S): Eli Lilly and Co., USA SOURCE: Brit. UK Pat. Appl., 40 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
GB 2121414	 A	19831221	GB 1983-15446		19830606
GB 2121414	В	19860305			
US 4552886	A	19851112	US 1983-472439		19830307
CA 1223586	A1	19870630	CA 1983-429587		19830602
DK 8302569	A	19831208	DK 1983-2569		19830606
EP 97013	A2	19831228	EP 1983-303256		19830606
EP 97013	А3	19850102			
R: BE, CH, DE,	FR, GE	B, IT, LI,	LU, NL, SE		
JP 59001481	A	19840106	JP 1983-101597		19830606
BR 8302975	A	19840207	BR 1983-2975		19830606
ни 31956	A2	19840628	HU 1983-2019		19830606
HU 193491	В	19871028			
PRIORITY APPLN. INFO.:			US 1982-385602	А	19820607
			US 1983-472439	А	19830307
OTHER SOURCE(S):	CASREA	CT 100:191	866: MARPAT 100:191866	s s	

OTHER SOURCE(S): CASREACT 100:191866; MARPAT 100:191866

ED Entered STN: 08 Jun 1984

AB The title compds. I [X = 0, S; X1 = bond, (un)substituted CH2, CH2CH2; R = pyridyl, pyrimidinyl, pyrazinyl, pyridazinyl; R1 = (un)substituted alkyl, Ph, alkenyl, alkoxy, cycloalkyl; R2-R4 = H, alkyl; n = 0, 1] were prepared Thus II (R5 = H) was treated with CH2:CHCH2NCS to give II (R5 = CSNHCH2CH:CH2) which was cyclized with acid to III. At 10 ppm III gave 86% growth inhibition of Hydrilla verticillata. At 35 lb/acre II protected cotton against damping off by Rhizoctonia.

IT 89985-33-1P

RN 89985-33-1 HCAPLUS

CN Benzonitrile, 4-[(4,5-dihydro-2-thiazolyl)(3-pyridinylmethyl)amino]- (CA INDEX NAME)

L44 ANSWER 24 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1980:198402 HCAPLUS Full-text

DOCUMENT NUMBER: 92:198402

ORIGINAL REFERENCE NO.: 92:32143a,32146a

TITLE: Substituted 2-phenylamino-2-imidazolines

INVENTOR(S): Staehle, Helmut; Koeppe, Herbert; Kummer, Werner;

Hoefke, Wolfgang

PATENT ASSIGNEE(S): Boehringer, C. H., Sohn, Fed. Rep. Ger.

SOURCE: Ger. Offen., 14 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KIND		DATE		AP:	APPLICATION NO.				DATE
							_							_	
	DE	2831	143			A1		1980	0131	DE	1978	-28311	.43		19780715
	ΕP	7986				A1		1980	0220	EP	1979	-10192	: 4		19790613
	ΕP	7986				В1		1981	0916						
		R:	AT,	BE,	CH,	DE,	FR	, GB,	ΙΤ,	LU, N	L, SE				
	ΑT	225				Τ		1981	1015	AT	1979	-10192	: 4		19790613
	JΡ	5501	5482			Α		1980	0202	JP	1979	-89179)		19790713
	US	4239	764			Α		1980	1216	US	1979	-57582			19790716
PRIOF	RITS	APP	LN.	INFO	. :					DE	1978	-28311	.43	Α	19780715
										EP	1979	-10192	: 4	Α	19790613

MARPAT 92:198402 OTHER SOURCE(S):

ED Entered STN: 12 May 1984

GΙ

AΒ The title compds. (I; R = H, Cl, Me, OMe; R1 = Cl, Me, Br, F, OMe, CN) and their salts were prepared for use as heart stimulants (no data). Thus, 2-(2,6-dichlorophenylimino)imidazolidine reacted with 2- (chloromethyl)pyridine-HCl in MeOCH2CH2OH to give I (R = Cl, R1 = 6-Cl, 2-pyridyl).

ΙT 73541-29-4P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

73541-29-4 HCAPLUS RN

Benzonitrile, 4-[(4,5-dihydro-1H-imidazol-2-yl)(2-pyridinylmethyl)amino]-CN (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

L44 ANSWER 25 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1978:406323 HCAPLUS Full-text

DOCUMENT NUMBER: 89:6323

ORIGINAL REFERENCE NO.: 89:1087a,1090a

TITLE: Substituted 2-phenylaminoimidazolines

INVENTOR(S): Staehle, Helmut; Koeppe, Herbert; Kummer, Werner; Stockhaus, Klaus; Hoefke, Wolfgang; Kuhn, Franz Josef

PATENT ASSIGNEE(S): Boehringer, C. H., Sohn, Fed. Rep. Ger.

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2636732	A1	19780216	DE 1976-2636732	19760814
FI 7702221	A	19780215	FI 1977-2221	19770718
FI 64147	В	19830630		
FI 64147	С	19831010		
AT 7705689	A	19791115	AT 1977-5689	19770802
AT 357152	В	19800625		
JP 53025567	A	19780309	JP 1977-94252	19770808
JP 60026112	В	19850621		
SU 660592	A3	19790430	SU 1977-2509800	19770810
DD 132964	A5	19781122	DD 1977-200535	19770811
СН 630906	A5	19820715	СН 1977-9858	19770811
BE 857778	A1	19780213	BE 1977-180163	19770812
DK 7703595	A	19780215	DK 1977-3595	19770812
DK 152042	В	19880125		
DK 152042	С	19880620		
NO 7702825	A	19780215	NO 1977-2825	19770812
NO 145275	В	19811109		
NO 145275	С	19820217		
SE 7709158	A	19780215	SE 1977-9158	19770812
SE 441184	В	19850916		
SE 441184	С	19860109		
NL 7708910	A	19780216	NL 1977-8910	19770812
FR 2361371	A1	19780310	FR 1977-24921	19770812
FR 2361371	B1	19800912		
US 4100292	A	19780711	US 1977-824044	19770812
ZA 7704875	A	19790425	ZA 1977-4875	19770812
GB 1548518	A	19790718	GB 1977-34025	19770812
ни 175055	В	19800528	HU 1977-B01676	19770812
CS 199686	В2	19800731	CS 1977-5341	19770812
CA 1085861	A1	19800916	CA 1977-284610	19770812
IL 52717	A	19801231	IL 1977-52717	19770812
ES 461598	A1	19780601	ES 1977-461598	19770813
PL 102537	В1	19790430	PL 1977-200251	19770813
PL 103477	B1	19790630	PL 1977-206252	19770813
RO 76806	A1	19810530	RO 1977-97261	19770813
AU 7727889	A	19790308	AU 1977-27889	19770815
AU 507063	B2	19800131	TO 1000 165005	40001000
ES 465225	A1	19780916	ES 1977-465225	19771220
SU 677655	A3	19790730	SU 1978-2611304	19780505
CS 199687	В2	19800731	CS 1979-903	19790209
AT 7904246	A	19801115	AT 1979-4246	19790615
AT 362787	В	19810610	OH 1001 F032	10010010
CH 631970	A5	19820915	CH 1981-5873	19810910
PRIORITY APPLN. INFO.:			DE 1976-2636732	A 19760814
			AT 1977-5689 CH 1977-9858	A 19770802
			CS 1977-5341	A 19770811 19770812
OTHER COHROL (C)	1120030	00 6000	00 19//-0041	19//0014

OTHER SOURCE(S): MARPAT 89:6323

ED Entered STN: 12 May 1984

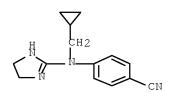
GI

AB The imidazoles I (R = R1 = R2 = halo, Me, Et, MeO, HO, CF3; n = 1-4) and their pharmaceutically acceptable salts were prepared by treating II with cycloalkylmethyl halides or III (R3 = CN, H2NC:NH, MeSC:NH, etc.), with H2NCHCHNH2. Thus, treating II (R = H, R1R2 = 2,6-Cl2) with (chloromethyl)cyclopropane gave 10.6% I (R = H, R1R2 = 2,6-Cl2, n = 1). I have analgesic activity up to 100 times that of morphine.

IT 66542-11-8P

RN 66542-11-8 HCAPLUS

CN Benzonitrile, 4-[(cyclopropylmethyl)(4,5-dihydro-1H-imidazol-2-yl)amino]-(CA INDEX NAME)



L44 ANSWER 26 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1974:120944 HCAPLUS Full-text

DOCUMENT NUMBER: 80:120944

ORIGINAL REFERENCE NO.: 80:19471a,19474a

TITLE: [(Furylmethyl)amino]imidazolines

INVENTOR(S): Stahle, Helmut; Koppe, Herbert; Kummer, Werner; Wick,

Helmut

PATENT ASSIGNEE(S): Boerhinger Ingelheim G.M.B.H.

SOURCE: Brit., 11 pp.
CODEN: BRXXAA

CODEN: BRAX

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

GB 1344022 19740116 GB 1972-29635 19720623 PRIORITY APPLN. INFO.: GB 1972-29635 A 19720623

Entered STN: 12 May 1984

GΙ For diagram(s), see printed CA Issue.

AΒ Twenty-one title compds. (I; R = H, Me, Et; R1, R2, R3 = H, F, C1, Br, Et, MeO, CF3, CN) which have analgesic and blood pressure decreasing properties and are useful in migraine treatment, were prepared by alkylation of the corresponding (phenylamino)imidazoline derivs. with (chloromethyl)furans or by treating appropriate N-phenyl-N-(furylmethyl)-S- methylisothiouronium iodides with H2N(CH2)2NH2. Thus, 2.3 g 2-(2,6-dichlorophenylamino)-2-imidazoline, 1.43 g 3-(chloromethyl)-2- methylfuran, and 3 ml Et3N were refluxed 3 hr in PhMe to give 1.95 g 2- N-(2-methyl-3-furylmethyl)-N-(2,6-dichlorophenyl)amino%-2- imidazoline. I-containing compns. for tablets, ampuls, and drops were described.

50531-23-2P ΤТ

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 50531-23-2 HCAPLUS

Benzonitrile, 4-[(4,5-dihydro-1H-imidazol-2-yl)]((2-methyl-3-CN furanyl)methyl]amino]- (CA INDEX NAME)

L44 ANSWER 27 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1974:463628 HCAPLUS Full-text

DOCUMENT NUMBER: 81:63628

ORIGINAL REFERENCE NO.: 81:10141a,10144a

TITLE: Analgesic and antihypertensive 2-anilinoimidazolines INVENTOR(S): Staehle, Helmut; Koeppe, Herbert; Kummer, Werner;

Hoefke, Wolfgang

PATENT ASSIGNEE(S): Boehringer, C. H., Sohn SOURCE:

Ger. Offen., 24 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2259160	A1	19740606	DE 1972-2259160		19721202
AT 7309432	А	19750215	AT 1973-9432		19731109
AT 326118	В	19751125			
NL 7316405	A	19740605	NL 1973-16405		19731130
AU 7363091	A	19750605	AU 1973-63091		19731130
JP 49086365	A	19740819	JP 1973-134831		19731201
ES 421067	A1	19760401	ES 1973-421067		19731201
ES 421068	A1	19760416	ES 1973-421068		19731201
BE 808150	A1	19740604	BE 1973-138456		19731203
FR 2208671	A1	19740628	FR 1973-43033		19731203
PRIORITY APPLN. INFO.:			DE 1972-2259160	Α	19721202

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB Fifty-five imidazolines I (Rn = e.g. 2,6-C12, 2-F3C, 4,2,6-BrC12, 2,4-F2, 2,6-Et2, or 2,4-C1Me; R1 = R2 = H or C1-12alkyl, or R1 = R2 = C1-12 alkyl), useful as antihypertensives and analgesics, were prepared by alkylation of I (R1 = R2 = H).

IT 53292-36-7P 53292-37-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 53292-36-7 HCAPLUS

CN Benzonitrile, 4-[butyl(1-butyl-4,5-dihydro-1H-imidazol-2-yl)amino]- (CA INDEX NAME)

RN 53292-37-8 HCAPLUS

CN Benzonitrile, 4-[butyl(4,5-dihydro-1H-imidazol-2-yl)amino]- (CA INDEX NAME)

L44 ANSWER 28 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:3523 HCAPLUS <u>Full-text</u> DOCUMENT NUMBER: 80:3523

ORIGINAL REFERENCE NO.: 80:619a,622a

TITLE: 2-(Arylamino)-2-imidazolines

INVENTOR(S): Merz, Herbert; Langbein, Adolf; Wick, Helmut;

Stockhaus, Klaus

PATENT ASSIGNEE(S): Boehringer, C. H., Sohn SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2208434	A1	19730830	DE 1972-2208434		19720223
DE 2208434	C2	19820916			
US 3850926	A	19741126	US 1972-282357		19720821
FR 2172948	A1	19731005	FR 1972-30915		19720831
PRIORITY APPLN.	INFO.:		DE 1971-2102733	A	19710121

US 1972-219535 A2 19720120 DE 1972-2208434 A 19720223

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB Thirty-two imidazolines I (Rn = 2,6-Cl2, 4,2- or 2,6-ClMe, 2-F3C, 2,4,6-Br3, etc.; R1 = CMe:CH2, 2-methyl-3-furyl, etc.) and(or) their salts, e.g. hydrochlorides, useful as analgesics and antihypertensives, were prepared either by alkylation of the amines II (or their metal salts) with R2CH2R1 (R1 = Cl, etc.) in the presence of bases, e.g. Et3N, or by condensation of RnC6H5- nN(CH2R1)R3 [R3 = CN or C(:NH)R4 with R4 = alkoxy, alkylthio, SH, or NH2] with H2NCH2CH2NH2.

IT 50531-23-2P

RN 50531-23-2 HCAPLUS

CN Benzonitrile, 4-[(4,5-dihydro-1H-imidazol-2-yl)](2-methyl-3-furanyl)methyl]amino]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NC} \\ \text{NH} \end{array}$$

L44 ANSWER 29 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1974:134887 HCAPLUS Full-text

DOCUMENT NUMBER: 80:134887

ORIGINAL REFERENCE NO.: 80:21761a,21764a

TITLE: Triphenylmethane dyes containing bis(trifluoromethyl)amino groups

AUTHOR(S): Dronkina, M. I.; Yagupol'skii, L. M.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1973), 9(10), 2167-72

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal LANGUAGE: Russian ED Entered STN: 12 May 1984

In styryl and triphenylmethane dyes the N(CF3)2 group has a weak auxochromic effect; analogs of crystal violet with 1, 2, and 3 NMe2 groups replaced by N(CF3)2 groups have λ max (98% H2SO4) 466, 474, and 470 nm, resp. 2-[P-[bis(trifluoromethyl)amino]styryl]benzothiazole (I) [50978-84-2] has λ max 325 nm, and its methiodide [50978-83-1] 366 nm. Amination of p-chloro-N,N-bis(trifluoromethyl)aniline (II, R = Cl) [10218-92-5] gave the diamine (II, R = NH2) [3700-30-9], which was converted via the Sandmeyer reaction to II (R = Br, iodine). By Grignard reaction of these with Et formate [109-94-4] was obtained 4,4'-bis[bis(trifluoromethyl)amino]benzhydrol [50978-82-0] which was oxidized with CrO3 to 4,4-bis[bis(trifluoromethyl)amino]benzophenone (III) [50978-81-9]. Further Grignard reaction of various combinations of III, Michlers ketone [90-94-8], II (R = halo), and p-BrC6H4NMe2 gave the crystal violet analogs.

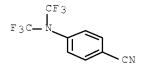
IT 51167-57-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 51167-57-8 HCAPLUS

CN Benzonitrile, 4-[bis(trifluoromethyl)amino]- (CA INDEX NAME)



L44 ANSWER 30 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1971:480250 HCAPLUS <u>Full-text</u>
DOCUMENT NUMBER: 75:80250

DOCUMENT NUMBER: 75:80250

ORIGINAL REFERENCE NO.: 75:12697a,12700a

Pharmacologically active substituted N-aminoalkyl TITLE:

arylamino-2-imidazolines

INVENTOR(S): Staehle, Helmut; Koeppe, Herbert; Kummer, Werner;

Samtleben, Hans W.

Boehringer, C. H., Sohn PATENT ASSIGNEE(S):

SOURCE: Ger. Offen., 27 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1957722	 A	19710519	DE 1969-1957722	19691117
DE 1957722	C3	19790628		
DE 1957722	В2	19781102		
СН 549575	A	19740531	СН 1973-3600	19701112
СН 550176	A	19740614	CH 1970-16781	19701112
CH 550177	A	19740614	СН 1973-3599	19701112
SU 386514	A3	19730614	SU 1970-1494776	19701113
SU 399128	A3	19730927	SU 1970-1724956	19701113
SU 402215	А3	19731012	SU 1970-1725405	19701113
SE 368010	В	19740617	SE 1970-15378	19701113
RO 58066	A1	19750615	RO 1970-67028	19701113
RO 58065	A1	19750715	RO 1970-67027	19701113
NL 7016744	A	19710519	NL 1970-16744	19701116
NL 169470	В	19820216		
NL 169470	С	19820716		
ES 385586	A1	19730316	ES 1970-385586	19701116
US 3752810	A	19730814	US 1970-90036	19701116
GB 1330887	A	19730919	GB 1970-54473	19701116
DK 130410	В	19750217	DK 1970-5817	19701116
PL 81165	B1	19750830	PL 1970-144454	19701116
FR 2073369	A1	19711001	FR 1970-41116	19701117
FR 2073369	A5	19711001		
AT 298484	В	19720510	AT 1970-10346	19701117
AT 300790	В	19720810	AT 1971-5147	19701117
AT 300791	В	19720810	AT 1971-5148	19701117
ES 388480	A1	19740116	ES 1971-388480	19710220
ES 388481	A1	19740116	ES 1971-388481	19710220
JP 49017265	В	19740427	JP 1972-65867	19720630
SE 415758	В	19801027	SE 1973-7442	19730225

Page 314 of 318

DK 132077 B 19751020 DK 1974-325 19740122 DK 7502612 A 19750915 DK 1975-2612 19750610 DK 134519 B 19761122 PRIORITY APPLN. INFO.: DE 1969-1957722 A 19691117

DE 1969-1957/22 A 19691117 DK 1970-5817 A 19701116

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) were mainly prepared by alkylation of I (R = R1 = H). Only R was displaced. Thus, from I (Ar = 2,4-Cl(Me)C6H3, R = R1 = H), O(CH2CH2)2NCH2CH2Cl.HCl, and Na2CO3 in MeOCH2CH2OH there was obtained I (Ar = 2,4-Cl(Me)C6H3, R = O(CH2CH2)2NCH2CH2, R1 = H). In this manner .apprx.100 other I were prepared

IT 34397-09-6P

RN 34397-09-6 HCAPLUS

CN Benzonitrile, 4-[(4,5-dihydro-1H-imidazol-2-yl)[2-(4-morpholinyl)ethyl]amino]- (CA INDEX NAME)

L44 ANSWER 31 OF 31 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1972:3754 HCAPLUS Full-text

DOCUMENT NUMBER: 76:3754
ORIGINAL REFERENCE NO.: 76:662h,663a

TITLE: Syntheses in the 2-aminoimidazoline series

AUTHOR(S): Staehle, Helmut; Pook, Karl H.

CORPORATE SOURCE: Wiss. Abt., Firma C. H. Boehringer Sohn,

Ingelheim/Rhein, Fed. Rep. Ger.

SOURCE: Justus Liebigs Annalen der Chemie (1971), 751, 159-67

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal LANGUAGE: German ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB Reaction of 2-anilino-2-imidazolines with C1(CH2)nNR1R2 gave the corresponding 2-[N-phenyl-N-(amino-alkyl)amino]-2-imidazolines (I), which were isomers of 1-(aminoalkyl)-2-anilino-2-imidazolines. These were prepared independently from N-phenyl-S-methylisothiuronium salts and H2NCH2CH2NH(CH2)nNR1R2.

IT 34397-09-6P

RN 34397-09-6 HCAPLUS

CN Benzonitrile, 4-[(4,5-dihydro-1H-imidazol-2-yl)[2-(4-morpholinyl)ethyl]amino]- (CA INDEX NAME)

$$\begin{array}{c|c}
 & H & N \\
\hline
 & N \\
\hline
 & CH_2 - CH_2 - N \\
\hline
 & CN
\end{array}$$

Search History

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L3
          774 SEA SSS FUL L1
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L21
             STRUCTURE UPLOADED
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L22
L23
            0 SEA SSS SAM L16 AND L21
L24
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L25
            0 SEA SSS SAM L24 AND L21
            0 SEA SSS SAM L24 AND L16 AND L21
L26
    FILE 'HCAPLUS' ENTERED AT 10:13:42 ON 26 SEP 2008
L27
          62 SEA ABB=ON PLU=ON TURNBULL P?/AU
L28
           17 SEA ABB=ON PLU=ON CADILLA R?/AU
           675 SEA ABB=ON PLU=ON COWAN D?/AU
          250 SEA ABB=ON PLU=ON LARKIN A?/AU
L30
           71 SEA ABB=ON PLU=ON KALDOR I?/AU
L31
          479 SEA ABB=ON PLU=ON STEWART E?/AU
L32
         1513 SEA ABB=ON PLU=ON (L27 OR L28 OR L29 OR L30 OR L31 OR L32)
L33
            6 SEA ABB=ON PLU=ON L33 AND (L4 OR L17 OR L13)
L34
    FILE 'WPIX' ENTERED AT 10:15:27 ON 26 SEP 2008
L35
          10 SEA SSS SAM L8
L36
           109 SEA SSS FUL L8
L37
            2 SEA ABB=ON PLU=ON L36/DCR
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L38		2 SEA ABB=ON PLU=ON L33 AND L37
L39 L40	FILE	'BEILSTEIN' ENTERED AT 10:16:52 ON 26 SEP 2008 0 SEA ABB=ON PLU=ON L9 0 SEA ABB=ON PLU=ON L9
L41 L42	FILE	'HCAPLUS, WPIX' ENTERED AT 10:21:37 ON 26 SEP 2008 6 DUP REM L34 L38 (2 DUPLICATES REMOVED) 31 SEA ABB=ON PLU=ON (L13 OR L7 OR L4) NOT L34
L43	FILE	'WPIX' ENTERED AT 10:23:24 ON 26 SEP 2008 0 SEA ABB=ON PLU=ON L37 NOT L38
L44	FILE	'HCAPLUS' ENTERED AT 10:24:44 ON 26 SEP 2008 31 DUP REM L42 L43 L40 (0 DUPLICATES REMOVED)